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Submitted date: 06/05/2019 • Posted date: 06/05/2019

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Citation information: Rao, Davuluri Yogeswara; Anoop, Anakuthil (2019): Computational Study of Tandem C-C Coupling and C-H Activation Reaction of a Flexible Substrate. ChemRxiv. Preprint.

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Computational Study of *tandem* C-C Coupling and C-H Activation Reaction of a Flexible Substrate

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Keywords: Intramolecular Heck reaction, C-H Activation, Computational study, Reaction mechanism

Abstract

We carried out an extensive density functional theory calculations on the Pd catalyzed intramolecular Heck reaction followed by C-H activation of a brominated diene, (*Z*)-1-bromo-5-methyl-1,2-diphenylhexa-1,5-dien-3-ol, that yields fused cyclopentane. Accounting for the flexibility of the substrate, we have selected eight conformations using a combination of conformation search and modeling. Coordination of the catalyst (PdPPh₃) on the *re* and *si* faces of substrate generated 16 catalyst-substrate complexes. The bidentate complexes that has coordination from both the double bonds of the substrate is more stable than the corresponding monodentate complexes. The barriers for oxidative addition are 7.6-15.2 kcal

mol⁻¹; the monodentate complexes are in general more reactive with lower activation free energies. The next step, migratory insertion, is regioselective. The selectivity is correlated with the unique geometric features of the intermediates. In the *twisted* orientation, Pd-C1 and C5-C6 bonds are perpendicular to each other while these bonds are parallel in *eclipsed* ones. The *twisted* orientations facilitate 5-*exo* and 6-*endo* cyclization during the migratory insertion, whereas the *eclipsed* orientation allows only 5-*exo* cyclization. The 5-*exo* route have much lower activation free energies, in agreement with the experiments. To identify the most favourable pathways among the many proposed mechanisms for the C-H activations in similar *tandem* reactions, we have analyzed these pathways. The next step in 5-*exo* pathways is the C-H activation where *ortho*-H of phenyl group moves to Pd. This may happen directly or after the exchange of Br⁻ with HCO₃⁻. Among the four conformations analyzed, the latter pathway has lower activation free energies for three of them. The other way to compare the path is to compare the energies of the transition states. In this way, the former direct pathway is more favourable for three conformations. The next important step is the second C-C bond formation. Here also we analyzed three pathways different in the oxidation state and coordination at Pd centre. Comparing these pathways on stepwise barriers, each of the conformations have different favourable pathways. But on comparing the energies of the transition states, the most favourable path is the base-assisted pathway for three conformations. The major takeaway from this extensive analysis is that various conformations of a flexible substrate have different characteristic reaction profiles which makes it difficult to conclude on the choice of pathways. It is crucial to take care of the conformational flexibility.

Introduction

Heck reaction or Mizoroki-Heck reaction, the palladium catalyzed vinylation of organic halides (or triflates), is one of the most versatile and convenient method for forming carbon–carbon bonds at unsubstituted vinylic positions^{1–5}. The intramolecular version of Heck reaction is specifically attractive due to their entropy economy and the carbocyclic product scope^{6,7}. In recent years, *tandem* Heck coupling and C-H activation gained interest due to their atom economy and step economy.^{8–10} Understanding the mechanism of these cascade reactions is crucial for the future development of rational design.

Recently, J. K Ray and coworkers have reported Pd-catalyzed intramolecular Heck cyclization on halogenated diene scaffolds undergoing various mode of cyclization and termination leading to the formation of structurally differing fused cyclopenta(e)none and aromatic analogue¹¹. Although we have provided our preliminary computational results, a detailed computational study was necessary to appreciate the complexity involved in the mechanism of these *tandem* reactions. Among the reported reactions, some of the substrates can have highly complex reaction mechanisms. The conformational flexibility of the substrate with rotatable phenyl rings and flexible side-chain creates the first level of complexity. In addition, the *tandem* reactions have enhanced complexity with the possibility of many intertwined pathways in the catalytic cycle.

Computational studies on *tandem* Heck coupling and C-H activation reactions is rare^{12,13} although there are numerous experimental studies and theoretical studies for selected steps.¹⁴ While the studies on the selected steps are intended to solve specific problems and can bring in certain insights, the study of the whole is expected to give a comprehensive understanding. In the current article, we are presenting the detailed study on the Pd catalyzed *tandem* cyclisation reaction of (*Z*)-1-bromo-5-methyl-1,2-diphenylhexa-1,5-dien-3-ol, **1** → **2** (Figure 1) using the Density Functional Theory based calculations. We analyzed the pathways for the formation of the experimentally found product as well as the other possible product. This

is one of the most comprehensive studies comprising four pathways, and more importantly considering many conformations of the substrate for the large part of the catalytic cycle.

Figure 1: The Reaction considered in this study

Methods

One of the highlights of this study is the exploration of the conformational space of the substrate. For this, we carried out an initial conformational search using RDKit¹⁵ with MMFF94¹⁶ forcefield for *S* isomer of the substrate. The geometries generated from RDKit was optimized with Turbomole program package employing BP86^{17–22} functional and def2-SVP²³ basis set along with the Resolution-of-the-Identity²⁴ approximation and third generation of dispersion correction with Beck-Johnson damping^{25,26}. This method, RI-BP86-D3BJ/def2-SVP, is sufficiently accurate and highly efficient. After selecting the important conformations of *S* isomers as described below in the results, we have modelled the *R* isomers of the selected conformations by changing the chirality at C3. These selected isomers were used for the study of the remaining steps in the cycle, rather than choosing one or a couple of conformations by chemical intuition.

We used Turbomole program for optimizations. We characterised all minima (zero imaginary mode) and transition states (one imaginary mode) using normal mode analysis with aforce module. The Gibbs free energy corrections were taken from these calculations. The mode of the transition state was further confirmed by intrinsic reaction coordinate²⁷ using DRC module of Turbomole. We used relaxed surface scan to go from the reactant or intermediate

geometry to the product or next intermediate geometry in each step. The end point of the scan was fully optimized. Using these two geometries as the end points, we have optimized the minimum energy path (MEP) followed by transition state search using Climbing Image Nudged Elastic Band^{28,29} (CI-NEB). We used DL-find³⁰ module in Chemshell³¹ program for relaxed surface scan and NEB with Turbomole interface. With help of this method we study all intermediate steps in the catalytic cycle for finding proper transition states. Further, we also performed individual transition state optimization with Turbomole using the TS geometry from CI-NEB.

Results and Discussions

The catalytic cycle of general Heck coupling reactions consists of mainly three steps; oxidative addition (OA), migratory insertion (MI) and β -hydride elimination (Figure 2). The reaction **1** $\rightarrow$ **2** shown in Figure 1 involves a *tandem* intramolecular Heck reaction and C-H activation. A Scheme of the pathways considered in our study is shown in Figure 3. The overall catalytic cycle starts with oxidative addition (**B**), followed by migratory insertion for the first C-C bond formation (**D**). The steps **A** to **D** are common for all Heck reactions.

There are many more possibilities in the *tandem* intramolecular Heck coupling followed by CH activation. There are two possibilities for the migratory insertion (step **D** in Figure 3) – 5-*exo* or 6-*endo* cyclization. We have studied the 5-*exo*-cyclization pathway that gives experimentally observed product as well as the other 6-*endo* pathway. The next step in the 5-*exo* pathway is C-H activation and a second C-C bond formation. We have studied the C-H activation occurring directly after the 5-*exo*-cyclization (**E**) and the other possibility where Br^- is replaced by H_2CO_3^- (**E'** also known as base-assisted pathway). Similarly for the second C-C bond formation through reductive elimination, we have studied three possibilities, **F**, **F'**, and **F''**, the pathways differing in the oxidation state and coordination at Pd. In the 6-*endo*

Figure 2: A General Catalytic cycle for Intramolecular Heck coupling

pathway, similar to the general Heck coupling in Figure 2, the β -hydride elimination is the next step.

Considering the flexibility of the substrate, we have selected a few conformations of the substrate with conformational analysis and modelling as described in the section below. We have computed the intermediates and transition states for all the selected conformations for the first two common steps, oxidative addition and migratory insertion. Thereafter, some of these conformations were filtered out based on factors such as the feasibility for continuing the reaction, similarity of intermediates of different pathways, large differences in the activation barriers for the some steps. At least two *R* isomers and two *S* isomers were included in the analyses of the remaining steps.

Conformational Analysis of Substrate

The effect of considering more than one conformation in the study of catalytic cycle is one of the major aspect of this article. Three rotatable bonds generate the conformational flexibility in our substrate. We carried out an initial conformational search using RDKit to understand

A) Complexation, B) Oxidative Addition, C) Coordination (*Eclipsed/Twisted*), D) Migratory Insertion(5-*exo*/6-*endo*), E) C-H Activation, F,F',F'') C-C bond formation, G) Product Formation, H) Reductive Elimination, I) Replace Br^- by HCO_3^- , J) H_2CO_3 assisted CH activation, K) H_2CO_3 Elimination, L) HBr Elimination, M) β -hydride Elimination

Figure 3: The pathways analyzed in this study for the reaction **1** $\rightarrow$ **2** (Figure 1)

the conformational space. We generated 50 conformations of *S* isomer and the geometries were further optimized at RI-BP86-D3BJ/def2-SVP level using Turbomole. These optimized geometries were analyzed for their similarity for finding the unique conformations.

These conformations can be grouped into a few clusters of similar geometries based on a few geometric parameters, the rotatable single bonds, C2-C3, C3-C4 and C4-C5. See Figure 4 for a schematic representation of the clustering. The rotation around C2-C3 generated two types of conformations differing in the orientation of the side-chain **R** (**R** = CH(OH)CH₂(=CH₂)CH₃), above or below the plane of stilbene double-bond (C1=C2). As the *R* isomer of one set and the *S* isomer of the other set will have similar environment for the reaction, we have taken only one of them to reduce computation.

Figure 4: A schematic representation of the selection of conformations for the study. The geometries generated by RDKit was clustered based on the C-C bond rotations. The selected sets are shown in the frames. In the final step, the enantiomers of the selected geometries were modelled.

The remaining conformations consists of three sets based on the rotation around C3-C4. One of these sets that has the **R'** (**R'** = CH₂(=CH₂)CH₃) pointing away from C1=C2 was excluded in our study because **R'** and C1=C2 are in *anti* arrangement and therefore is not

suitable for the subsequent C-C bond formation. The final basis for clustering is the rotation around C4-C5. There are two sets of geometries based on this parameter. We have included both sets. This hierarchical clustering – 1/2 from first step, 2/3 from second step, 2/2 in third step – results in four sets (2×2).

We selected one conformation from each of this clusters and arrived at four *S* conformations (**S1-S4**). We need to consider the *R* and *S* isomers, as the experiment was done with the racemic substrate. With the selected unique conformations of *S* isomer, we have modelled the *R* isomers by flipping the chirality at C3 carbon. These geometries were optimized at the same level, RI-BP86-D3BJ/def2-SVP to create four *R* isomers (**R1-R4**). Thus, we have identified eight substrate conformations as the unique conformations for our study. The relevant torsion angles and the relative energies are given in Table 1. We assume that these eight conformations cover the possible range of conformational space and used them as the substrates for studying the catalytic cycle.

Table 1: Relative energies (ΔE^a ; kcal mol⁻¹) of the selected substrate isomers and their relevant torsion angles (in degrees), $\alpha \leftarrow (C1 - C2 - C3 - C4)$; $\beta \leftarrow (C2 - C3 - C4 - C5)$; $\gamma \leftarrow (C3 - C4 - C5 - C6)$; and $\theta \leftarrow (C1 - C2 - C5 - C6)$.

Xn	ΔE^a	α	β	γ	θ
R1	0.0	80.2	61.2	78.2	173.8
R2	0.3	80.1	50.2	-113.4	30.6
R3	1.7	101.9	-69.3	-94.3	-67.9
R4	0.7	100.1	-68.1	100.2	67.1
S1	2.1	76.7	50.2	76.9	157.2
S2	0.5	76.8	51.2	-110.9	29.3
S3	1.8	102.6	-73.0	-85.8	-70.0
S4	2.4	96.2	-65.9	96.4	61.6

To simplify our discussion, we will reduce the dimensionality by showing the differences

between the isomers by one representative dihedral angle ($\theta = \angle \text{C1-C2-C5-C6}$) which shows the angle between the two double bonds in the substrate. The double bonds point away from each other ($\theta = 173.8^\circ$ and 157.2°) in **R1** and **S1**. In **R2** and **S2**, the orientation of double bonds are similar to each other ($\theta = 30.6^\circ$ and 29.3°). In the others, **R3**, **S3**, **R4**, and **S4** the angle between the double bonds are around 60 degrees.

The energies of all the conformations (**Xn**; **X** = *R* or *S*, **n** = **1-4**) are within ~ 2 kcal mol⁻¹. The difference in their energies can be attributed to various noncovalent interactions such as, CH $\cdots\pi$, CH $\cdots$ O and O-H $\cdots\pi$ interactions, among the phenyl, -CH, and -OH groups. These interactions are schematically shown in Figure 5, the detailed analysis using non-covalent index (NCI) is given in the supporting information. Choosing any one among these energetically similar conformations is difficult and non-intuitive. Thus we included all eight conformations in the study.

Complexes of the Active Catalyst with Substrates (**A**)

We proceeded to the catalytic cycle with these eight selected substrate isomers. The catalyst will form a π -complex with the substrate through the double bond (C1=C2) prior to the oxidative addition (OA) step. Thus, we first modelled the substrate-catalyst complexes (**A**). The mostly recommended³²⁻³⁶ active catalyst model PdL (L = triphenylphosphine), mono ligated palladium catalyst was chosen as the catalyst in this work. We have considered the two possibilities of π -complexes where PdPh₃ is coordinated to one of the two faces (*re* and *si*) of C1=C2 double bond.

In the optimized geometries where Pd and the side-chain are in the same side of the olefinic plane, a bidentate complex is formed by the coordination of both the double bonds. We will include **B** to the name of these substrate conformation to indicate the bidentate coordination of substrate to the complex (e.g. **BR1** is the catalyst-substrate complex with PdL coordinated with the substrate **R1**). The optimized geometries are shown in Figure 6. In the other set of

Figure 5: Optimized geometries of the selected conformations of the substrate, $[\mathbf{R}, \mathbf{S}][1-4]$

complexes, the Pd and the side-chain are on the opposite side of the olefinic plane. Therefore PdL is coordinated monodentatively to C1=C2. These complexes are named with **M** to indicate the monodentate coordination (e. g., **MR1**).

The complexation (Step A in Figure 3) is exergonic for both monodentate ($\Delta G^A = -29.7$ to -32.2 kcal mol⁻¹) and bidentate (-36.8 to -43.2 kcal mol⁻¹) coordination (Table 2). The complexation energy (ΔG^A) is calculated as the energy difference between the complex and the sum of the energies of the free substrate and PdL. The bidentate complexes **BXn** (**X** = **R** or **S**, n = 1-4) are more stable with the stabilization from an additional coordination and extra stabilization from chelation compared to monodentate complexes.

Table 2: Relative energies (ΔE^a ; kcal mol⁻¹), complexation energies (ΔG^A) and the relevant torsion angles ($\theta \leftarrow (C1-C2-C5-C6)$; in degrees) of bidentate (**BXn**) and monodentate (**MXn**) complexes. The ΔE^a 's are calculated with reference to **MR1a** for monodentate complexes and **BR1a** bidentate complexes.

MX _n a	θ	ΔE^a	ΔG^A	BX _n a	θ	ΔE^a	ΔG^A
R1	166.4	0.00	-29.73	R1	125.0	0.00	-37.25
S1	159.2	-0.64	-31.63	S1	122.8	-2.80	-42.44
R2	31.2	1.01	-29.95	R2	15.6	-1.00	-36.79
S2	27.4	-2.30	-32.19	S2	16.2	-5.01	-41.25
R3	-73.1	1.16	-30.07	R3	-22.5	-3.63	-41.01
S3	-74.1	-0.30	-31.39	S3	-28.3	-3.14	-41.39
R4	64.5	-0.33	-30.47	R4	87.0	-6.63	-43.17
S4	60.4	-0.6	-31.88	S4	181.3	-2.05	-41.67

The range of relative energies among the **MXn** is ~ 2.5 kcal mol⁻¹, slightly more than their spread in substrate conformations (~ 2 kcal mol⁻¹). The order of relative energies has changed – while **MS2a** is the most stable complex, **R1** is the most stable substrate. Such variations are expected as the interactions of substrate functional groups with the phenyl groups of the

Figure 6: Optimized geometries of bidentate catalyst-substrate complexes $\mathbf{B[R,S][1-4]a}$

ligand may stabilize some conformations more than the others.

The spread of energies in **BXn** are more, 6.4 kcal mol⁻¹, than in **MXn** and in substrates. The magnitude of interactions among the functional groups, attractive or repulsive, are higher as the groups come closer in the bidentate coordination. The difference in ring-strain for different cyclic arrangements also may contribute the variations in relative energies. These variations also changes the ordering of energies. The most stable substrate **R1** lead to the least stable bidentate complex **BR1a**. There are various geometric factors that affect the relative energies, however, none of these takes a dominant role as we observe no particular trends in the relative energies.

The bidentate complexes of **1** and **4** conformations (**BR1a**, **BS1a**, **BR4a**, and **BS4a**) have the *si* face of C5=C6 coordinated with Pd. The angle (θ) that represent the relative orientation of double bonds in **1** and **4** conformations are $>81.3^\circ$. We refer to this as *twisted* complexes considering the nearly perpendicular relative orientations of double bonds. In contrast, the complexes of **2** and **3** conformations have a *re* face coordination of C5=C6 with Pd. The θ in **2** and **3** are $<22.5^\circ$. We refer to them as *eclipsed* complexes. Coordination of *si* face gives *twisted* and the coordination of *re* face gives *eclipsed* complexes.

Generally, the perpendicular orientation of *trans* olefins are more stable than the parallel orientation in π -coordinated *bis*-olefinic metal complexes.³⁷ The *twisted* complex **BR4a** with $\theta = 87.0^\circ$ is most stable. The stabilization from this factor, however, is not found in the similar **BS4a** with $\theta = 81.250^\circ$ that is less stable than **BR4a** by ~ 4 kcal mol⁻¹.

Another difference between the complexes is the chirality at C3 carbon containing the OH group. In two of the *S* complexes, **BS3a** and **BS4a**, we can see the OH—Br interactions that will give some extra stability. The varying stabilizations from the interactions among the aromatic groups in stilbene and triphenylphosphine also bring variations in the relative stabilities.

Although the **MXna** complexes are at least 7 kcal mol⁻¹ less stable than the corresponding

BXna complexes we included both types because of their high complexation energies ($> 30 \text{ kcal mol}^{-1}$). We studied the oxidative addition with these 16 geometries.

Oxidative Addition (B)

We have studied the oxidative addition (OA; step B in Figure 3) with all the 16 substrate-catalyst complexes, **[M, B][R, S][1-4]a**. In this step, the Pd is inserted into the Pd-C1 bond. The associated changes in the geometry are: the Pd moves from the π -coordination with C1=C2 bond to form the Pd-C1 bond, Br migrates from C1 to Pd, and the C5=C6 (the double-bond of the side chain) slightly moved away from the Pd weakening the π -coordination of Pd with C5=C6.

The activation free energies ($\Delta^\ddagger G^B$; Table 3) vary between 8.7-15.2 kcal mol $^{-1}$ for **BXn** and 7.6-9.5 kcal mol $^{-1}$ for **MXn**. The lower step-wise barriers for **MXn** compared to those for **BXn** are due to higher relative energies of **MXna**. The transition states corresponding to **BXn** are more stable than those of **MXn**. Thus, the relatively less stable **MXna** substrate-catalyst complexes are more reactive with a relatively lower barriers compared to the **BXna** complexes.

Table 3: Free energies of activation ($\Delta^\ddagger G^B$) and reaction ($\Delta^r G^B$) for oxidative addition (**a** $\rightarrow$ **b**; in kcal mol $^{-1}$).

MXna	$\Delta^\ddagger G^B$	$\Delta^r G^B$	BXna	$\Delta^\ddagger G^B$	$\Delta^r G^B$
R1	9.27	-21.06	R1	14.19	-8.64
S1	9.52	-22.82	S1	15.22	-9.29
R2	9.08	-20.58	R2	14.43	-2.50
S2	8.79	-22.11	S2	13.02	-5.79
R3	9.31	-21.07	R3	10.41	-6.06
S3	7.58	-22.61	S3	10.29	4.67

MXna	$\Delta^\ddagger G^B$	$\Delta^r G^B$	BXna	$\Delta^\ddagger G^B$	$\Delta^r G^B$
R4	8.17	-19.89	R4	9.82	-6.44
S4	8.39	-20.80	S4	8.71	1.25

The smallest step-wise barrier for the OA step is for **MS3a** (7.58 kcal mol⁻¹) and the most stable TS geometry is that of **BR4a**. The largest step-wise barrier is for **BS1a** (15.22 kcal mol⁻¹) and the least stable TS is that of **BR1a** (10.2 kcal mol⁻¹ higher). The large range of values (~6 kcal mol⁻¹) for the activation free energies further justify the importance of conformational sampling for estimating the accurate rate of the reaction for substrates with large conformational space.

After the oxidative addition in bidentate complexes (**BXn**), the geometries of intermediates corresponding to the isomers **R1**, **R4**, **S3** and, **S4** have retained the π -coordination from C5=C6, the olefin of the side-chain, while the C5=C6 moved away from Pd-centre and resulted in a T-shaped geometry, i. e., square-planar with a vacant site at Pd(II)-centre. The other notable changes are in the intermediates **BS3b** and **RS4b** that has OH $\cdots$ Br interaction, the Br moved away from Pd. This intermediate (**b**) will be rearranged to facilitate the migratory insertion.

Coordination of the Second Double Bond to Pd (C)

The second double bond, C5=C6, has to be coordinated with Pd to facilitate migratory insertion. This rearrangement (step **C**; **b** $\rightarrow$ **c** in Figure 3) is a minor change in geometry for **BR1**, **BR4**, **BS3** and, **BS4** where the π -coordination was preserved in oxidative addition step. The Pd-C5 and Pd-C6 distances before (d^{1b} and d^{2b}) and after (d^{1c} and d^{2c}) the rearrangement (C) is given in Table 4. In the other **BXnb** intermediates, the rearrangement will bring back the π -coordination from C5=C6. This rearrangement is exergonic in all cases.

Although the C5=C6 are relatively farther away from Pd in the monodentate intermediates, the coordination can be achieved in **MXnb** (n=3, 4). The major difference between the **BXnc** and **MXnc** is in the orientation of ligands around Pd. PPh₃ is in *cis* position with C1 in **MXnc** while PPh₃ is in *trans* position with C1 in **BXnc**.

Table 4: The Pd-C distances (in Å) before and after the rearrangement (C; **Xnb** $\rightarrow$ **Xnc**). $d^{1b} \leftarrow (Pd - C5)$ in **BXnb**, $d^{2b} \leftarrow (Pd - C6)$ in **Xnb**, $d^{1c} \leftarrow (Pd - C5)$, $d^{2c} \leftarrow (Pd - C6)$ in **Xnc**.

Xnb	d^{1b}	d^{2b}	ΔE^b	Xnc	d^{1c}	d^{2c}
BR1	2.12	2.11	6.09	BR1	2.16	2.17
BR2	4.54	4.79	13.20	BR2	2.31	2.17
BR3	3.63	3.38	7.26	BR3	2.36	2.17
BR4	2.23	2.18	3.77	BR4	2.24	2.17
BS1	4.14	4.90	2.39	BS1	2.23	2.16
BS2	3.74	3.78	4.24	BS2	2.37	2.17
BS3	2.64	2.27	17.35	BS3	2.37	2.17
BS4	2.41	2.24	13.95	BS4	2.27	2.17
MR1	4.66	5.88	2.15	MR1	—	—
MR2	4.78	4.97	3.04	MR2	—	—
MR3	3.59	3.64	3.85	MR3	2.54	2.28
MR4	3.92	3.40	3.58	MR4	2.37	2.23
MS1	5.64	6.51	13.02	MS1	—	—
MS2	3.98	4.18	11.03	MS2	—	—
MS3	4.34	4.67	0.00	MS3	2.55	2.28
MS4	3.98	4.18	2.41	MS4	2.41	2.24

The resulting complexes, **[B, M]Xnc**, are tetra coordinated Pd(II) complexes. We will now discuss the migratory insertion (MI; **D** in Figure 3) in the next section.

Figure 7: Optimized geometries of the intermediates, $B[R,S][1-4]c$, resulting from the oxidative addition (B) followed by rearrangements (C)

Migratory Insertion *aka* Carbopalladation (D)

The migratory insertion is the most important regioselective step that determine the products. This is the first diverging step in the catalytic cycle that can produce either 5-*exo* or 6-*endo* products. We calculated the reactions from 12 **c** intermediates – eight **BXnc** and four **MXnc** – leading to 18 **d** intermediates – 12 *exo* and 6 *endo*. Among all the stepwise activation free energies ($\Delta^\ddagger G^D$; Table 5), the lowest barriers are for the *exo* cyclizations ($\sim 4\text{-}6$ kcal mol⁻¹). The lowest barrier for *endo* cyclization is 20.8 kcal mol⁻¹ showing a clear preference for the products based on *exo*-cyclization, in support of the experimental observation.

Table 5: Free energy of activation ($\Delta^\ddagger G^D$) and reaction ($\Delta^r G^D$) of migratory insertion step in kcal mol⁻¹.

Xnc	product	$\Delta^\ddagger G^D$	$\Delta E^{D(TS)}$	$\Delta^r G^D$
BR1	<i>exo</i>	24.80	18.82	-8.67
BR1	<i>endo</i>	26.17	23.15	-13.78
BS1	<i>exo</i>	35.03	27.06	-2.56
BS1	<i>endo</i>	22.99	13.55	-6.01
BR2	<i>exo</i>	4.77	10.06	-19.74
BS2	<i>exo</i>	6.03	3.42	-26.19
BR3	<i>exo</i>	4.00	9.15	-16.57
BS3	<i>exo</i>	5.86	3.44	-23.07
BR4	<i>exo</i>	29.28	27.27	-5.95
BR4	<i>endo</i>	24.58	22.03	-8.84
BS4	<i>exo</i>	34.19	28.93	-3.02
BS4	<i>endo</i>	20.75	14.17	-5.15
MR3	<i>exo</i>	17.60	9.01	-2.97
MS3	<i>exo</i>	14.92	0.00	-2.53
MR4	<i>exo</i>	42.01	28.13	10.29

Xnc	product	$\Delta^\ddagger G^D$	$\Delta E^{D(TS)}$	$\Delta^r G^D$
MR4	<i>endo</i>	29.76	14.62	1.26
MS4	<i>exo</i>	47.98	29.07	15.87
MS4	<i>endo</i>	25.71	6.69	2.73

What makes *exo* pathways special? We can look at the geometries of the **c** intermediates of the low barrier paths, **BXnc**; **X** = *R*, *S*; **n** = 2, 3. All these low barrier paths are from bidentate-*eclipsed* intermediates (Figure 8). Only *exo* cyclizations are possible for them. The similar paths from monodentate-*eclipsed* paths, **MX3**, the $\Delta^\ddagger G^D$ for 5-*exo*-cyclization are 17.6 and 14.9 kcal mol⁻¹ for **MR3** and **MS3**, much higher than the **BXn** counterparts (4.0 and 5.9 kcal mol⁻¹). Although **MS3** has 14.9 kcal mol⁻¹ of step-wise barrier, it has the most stable transition state geometry among all the transition states in migratory insertion paths.

Figure 8: The orientation of C5=C6 in *twisted* and *eclipsed* **Xnc**-complexes

The *twisted* isomers of **1** and **4** conformations can undergo both cyclizations. Between the two possible cyclizations, the 6-*endo* cyclization is more favoured in all the cases except for **BR1c** where 5-*exo* pathway is slightly more favourable. The barriers $\Delta^\ddagger G^D$ for 6-*endo* cyclizations are in the range 21-26 kcal mol⁻¹. The *exo* cyclizations from *twisted* intermediates have much higher activation barriers ranging between 25-35 kcal mol⁻¹ for **B** pathways and 42 and 48 kcal mol⁻¹ for **M** pathways. Another observation is that the *S* pathways have higher barriers than *R* pathways in these *exo* cyclizations from *twisted* intermediates.

Some of the geometrical features of the **c** intermediates (Figure 7) can contribute to the

selectivity. A major reaction coordinate in this step is the approach of C5 to C1 for 5-*exo* and C6 to C1 for 6-*endo* cyclization. The distances, d^{3c} between C1 and C5 and d^{4c} between C1 and C6 are shown in Table 6. A representative geometric parameter that helps to identify the *twisted* versus *eclipsed* intermediates are the dihedral angles in $\theta^{1c} \leftarrow (C1 - C2 - C5 - C6)$ and $\theta^{2c} \leftarrow (C1 - Pd - C5 - C6)$.

Table 6: Bond distances between the coupling carbon atoms, $d^{3c} \leftarrow (C1 - C5)$, $d^{4c} \leftarrow (C1 - C6)$, $\theta^{1c} \leftarrow (C1 - C2 - C5 - C6)$, $\theta^{2c} \leftarrow (C1 - Pd - C5 - C6)$ in **Xnc**. The distances (d) are in Å and angle (θ) in degrees.

Xnc	d^{3c}	d^{4c}	θ^{1c}	θ^{2c}
BR1	3.00	2.88	66.06	-81.05
BR2	2.67	3.48	-32.99	-169.05
BR3	2.64	3.42	-56.63	-169.06
BR4	3.01	2.99	39.58	-92.17
BS1	3.00	2.99	39.68	-93.29
BS2	2.69	3.46	-54.86	-173.91
BS3	2.69	3.46	-54.84	-173.86
BS4	2.98	3.00	40.97	-94.76
MR3	2.83	3.50	-54.94	-176.65
MR4	3.09	3.03	32.52	-92.57
MS3	2.81	3.48	-53.33	-177.91
MS4	3.11	3.00	38.80	-90.70

The relative orientation of C5=C6 with Pd-C1 bond is nearly perpendicular in *twisted* intermediates of **1** and **4** conformations as can be seen from the dihedral angle C1-Pd-C5-C6 $\theta^{2c} = 81^\circ - 95^\circ$. Hence the C5 and C6 atoms, the carbon atoms that are going to couple with C1, are in similar distances from C1 (~ 3 Å). Thus, both 5-*exo* and 6-*endo* cyclization are possible from these intermediates. On the other hand in the *eclipsed* intermediates of **2** and **3** conformations, the C5=C6 bond is parallel to Pd-C1 bond ($\theta = 169^\circ - 178^\circ$). Thus in these cases, the C1 is close to C5 (~ 2.6 - 2.8 Å), but C6 is farther from C1 (~ 3.4 - 3.5 Å). This way, C5 flanks the approach of C1 to C6, and therefore only C1-C5 coupling is expected from these orientations. For these intermediates, the 6-*endo* cyclization is practically impossible without a major rearrangement of the complex.

All the MI steps from the **BXnc** intermediates are exergonic, while **MXnc** intermediates have endergonic MI steps. In the **BXnd** intermediates formed by the MI, the Pd orients such that the vacant coordination site generated by the MI step is satisfied by coordinating to an adjacent double bond, oxygen or bromine. In **BS2d'** and **BS3d'**, Pd gets coordinated to C1=C2 and have a OH $\cdots$ Br interaction as the OH and Br are on the same side of the ring. These are also the most stable among the four **d** intermediates formed from *eclipsed-c* intermediates. Similarly, **BR2d** and **BR3d** have similar geometry around the newly formed 5-membered-cycle. The methyl and hydroxyl groups are on the same side of the ring, both are on the opposite side of the CH₂PdL. Among the 5-*exo* intermediates formed from *eclipsed c* intermediates, **1** and **4** are similar.

The reaction profile for all the conformations for the steps upto the migratory insertion is shown in Figure 9. Comparing the geometries and energies of the intermediates formed by MI, we can find that the pathways corresponding to **2** and **3** have converged and similarly **1** and **4** pathways have converged. For the remaining part of the catalytic cycle, we chose **BR3d'**, **BS3d'**, **BR4d**, and **BS4d** intermediates. We discuss the 5-*exo* pathways first, the 6-*endo* pathway will be discussed at the end.

Figure 9: Reaction profile for all conformations for steps A-D

C-H Activation

The next step in the pathways for the formation of **2** (Figure 1) is the activation of C'-H in the *ortho*-position of the phenyl group that is adjacent to Pd. This can occur directly from the **d** intermediates formed by the 5-*exo* cyclization. The other possibility is the base assisted (or concerted metalation-deprotonation)³⁸⁻⁴⁰ pathway. We discuss these two possibilities below.

Direct C-H Activation from **d** (E)

In the four intermediates we considered for the subsequent steps, the Pd(II) is coordinated weakly with the adjacent phenyl ring in **BR4d** and **BS4d**, that is a suitable orientation for C-H activation. But, in **BR3d'** and **BS3d'**, the Pd is coordinated with stilbene (C1=C2) and would require a rearrangement before the C-H activation. This rearrangement is endothermic by 2.2 kcal mol⁻¹ for **BR3d'** and 10 kcal mol⁻¹ for **BS3d'**. The optimized structures of C-H coordinated complexes **BR4d**, **BS4d**, **BR3d**, and **BS3d** are presented in Figure 10 with their structural parameters. In all the **d** intermediates, the Pd(II) is coordinated to the nearest phenyl ring of the stilbene.

In the C-H activation, hydrogen migrates from carbon (C') to Pd(II) and forms the **e**-intermediates that has Pd(IV) centre with higher coordination number and oxidation state. The Pd(II) activates the C'-H bond in the *ortho*-position of the phenyl ring to which Pd is coordinated. The C-H activation is the important and rate determining step in the catalytic cycle.³⁸⁻⁴² In our calculations also this step (step E in Figure 3) has the highest step-wise activation barriers, ~27 kcal mol⁻¹, among all the other steps calculated so far (Table 7).

Figure 10: Optimized geometries of **d** intermediates formed by migratory insertion, followed by a rearrangement. The C'-H is coordinated to Pd in these complexes

Table 7: Free energies of activation and reaction ($\Delta^\ddagger G^E$ and $\Delta^r G^E$; in kcal mol⁻¹) for C-H activation.

BXnd	$\Delta^\ddagger G^E$	$\Delta^r G^E$
R3	27.63	23.36
S3	27.50	25.83
R4	27.51	24.92
S4	26.43	23.69

This step is highly endergonic. The optimized geometries of Pd(IV) complexes of **BR3e**, **BR4e**, and **BS4e** are presented in the Figure 11. The intermediates after the C-H activation of isomers **BR3e**, **BR4e**, and **BS4e** are octahedral Pd(IV)-complexes with one vacant site. The **BS3e** intermediate has a different geometry in which the fourth site of Pd(IV) is coordinated with oxygen of the OH group.

Base Assisted C-H Activation (E')

Base Assisted C-H Activation, also known as Concerted Metalation-Deprotonation (CMD), occurs after the bromide in the **d** intermediate is replaced by HCO₃⁻ (step I in Figure 3). This ligand exchange process (I) is endergonic by 11.2-20.6 kcal mol⁻¹ (Table 8).

Table 8: Free energy of reaction for Ligand exchange reaction ($\Delta^r G^I$), free energy of activation ($\Delta^\ddagger G^{E'}$) and reaction ($\Delta^r G^{E'}$) for base (H₂CO₃) assisted C-H bond activation. All Energies are in kcal mol⁻¹.

BXnd	$\Delta^r G^I$	$\Delta^\ddagger G^{E'}$	$\Delta^r G^{E'}$
R3	20.58	19.22	8.66
S3	13.04	30.12	17.97
R4	12.95	14.96	3.87
S4	11.27	17.34	10.45

BX _{nd}	$\Delta^r G^I$	$\Delta^\ddagger G^{E'}$	$\Delta^r G^{E'}$
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The C-H activation in this pathways is achieved by a different mechanism. The oxygen of the bicarbonate base takes the hydrogen from *ortho* position to form H₂CO₃ coordinated Pd(II) complex. Compared to the direct C-H activation (E) discussed above, this step (E') have significantly lower activation free energies ($\Delta^\ddagger G^{E'}$) except for **BS3d**. This step is much less endergonic compared to E (Table 8).

Although the barriers are lower for E' in three cases, this pathway involves an endergonic ligand exchange step, I. Thus it is worthy to compare the energies of transition states (**e** + H₂CO₃ versus **e'** + HBr). There is slight advantage for base-assisted E' path in **R4**, while for the other conformations, the direct E paths are more favourable than the E' path.

C-C reductive elimination

The C-C reductive elimination is the second C-C bond formation step that facilitate the formation of the second ring. We studied this step from three different types of intermediates, i) **e** in the direct path, ii) **e'** in which HBr is replaced by H₂CO₃, and iii) **j/k** where HBr or H₂CO₃ is eliminated. The Pd is coordinated, in addition to the substrate, by only PPh₃. The **e** is formed by direct C-H activation, whereas **e'** is formed by C-H activation after the replacement of HBr by H₂CO₃, and **j/k** is formed by the elimination of HBr from **e** (J), or elimination of H₂CO₃ (K) from **e'**.

The direct path (F)

The activation free energies ($\Delta^\ddagger G^F$) for this step is given in Table 9. The $\Delta^\ddagger G^F$ is considerably low for **BR3e** pathway (8.78 kcal mol⁻¹) among the corresponding barriers for the other isomers (17.20 - 22.33 kcal mol⁻¹). A closer look at the path using IRC shows a two step

Figure 11: Optimized geometries of $\bullet$ intermediates formed by CH Activation.

process, an initial movement of the PPh_3 ligand from a *cis* position with respect to sp^3 carbon (C6) to the *trans* position. This rearrangement from **BR3e** to **BR3e'** has a free energy barrier of $7.15 \text{ kcal mol}^{-1}$ and is endergonic by $1.37 \text{ kcal mol}^{-1}$. In **BR3e'**, the PPh_3 have stabilising interactions with phenyl groups of stilbene that lower the activation energy. The highest barrier among the pathways is for **BS3e** that can be attributed to the interaction with -OH and Pd which are in the same side of the ring that increases the strain in the transition state and hence increases the activation free energy ($22.33 \text{ kcal mol}^{-1}$). The C-C reductive elimination is exergonic in all the cases (Table 9).

Table 9: Free energy of Activation ($\Delta^\ddagger G^F$) and reaction ($\Delta^r G^F$) for C-C reductive elimination.

BXne	$\Delta^\ddagger G^F$	$\Delta^r G^F$
R3	8.78	-28.89
S3	22.33	-33.29
R4	17.20	-28.61
S4	19.48	-27.11

C-C Bond Formation (F') after HBr/H₂CO₃ Elimination (J/K)

In contrast to the direct pathway (F) discussed above where the HBr is removed after the C-C reductive elimination, the HBr or H₂CO₃ is eliminated in the F' path prior to the C-C reductive elimination. In the HBr elimination from **e**, first the H-Br bond is formed and the HBr remain coordinated with Pd. The dissociation of this complex in free **k** and HBr is endothermic with a dissociation energy ($\Delta^{diss.} G^K$; Table 10) of $6.9\text{-}10.6 \text{ kcal mol}^{-1}$. The elimination of HBr is fairly easy for **BS3** with a free energy of activation ($\Delta^\ddagger G^K$) of $6.7 \text{ kcal mol}^{-1}$, while $\Delta^\ddagger G^K$ is rather high for **BS4** ($19.5 \text{ kcal mol}^{-1}$). Similarly we have calculated the $\Delta^{diss.} G^J$ for the dissociation of H₂CO₃ from **e'**. The dissociation energy for H₂CO₃ is lower for **R3**, and higher for others.

Table 10: Free energies of activation ($\Delta^\ddagger G^K$) and reaction ($\Delta^r G^K$) for the elimination of HBr. The last column shows the $\Delta^{diss.}G$ for the dissociation into **j** + HBr.

BXne	$\Delta^\ddagger G^K$	$\Delta^r G^K$	$\Delta^{diss.}G^K$	$\Delta^{diss.}G^J$
R3	7.73	0.38	10.64	8.34
S3	6.71	0.06	6.91	11.54
R4	10.16	-0.84	7.38	17.01
S4	19.46	-0.05	6.85	10.72

Table 11: Free energies of activation for C-C reductive elimination ($\Delta^\ddagger G^{F'}$), and free energies of reaction for the C-C reductive elimination ($\Delta^r G^{F'}$) in **R3**, **S3**, **R4**, and **S4** pathways. All energies in kcal mol⁻¹.

BXnl	$\Delta^\ddagger G^{F'}$	$\Delta^r G^{F'}$
R3	13.80	-24.56
S3	10.63	-24.63
R4	15.05	-24.01
S4	17.43	-22.54

The free energies of activation ($\Delta^\ddagger G^{F'}$; Table 11) are 10.6-17.4 kcal mol⁻¹.

Base assisted C-C bond formation (**F''**)

In this pathway, **F''**, the C-C bond formation occurs from **e''** before the elimination of H₂CO₃.

This step has a barrier of 8.23 kcal mol⁻¹ for **S3** and ~17 kcal mol⁻¹ for the others.

Table 12: Free energy of Activation ($\Delta^\ddagger G^K$) and reaction ($\Delta^r G^K$) for base (H_2CO_3) assisted C-C reductive elimination.

BXne'	$\Delta^\ddagger G^{F''}$	$\Delta^r G^{F''}$
R3	16.31	-16.14
S3	8.23	-21.75
R4	17.53	-12.58
S4	17.42	-16.93

Comparing all the three pathways for C-C bond formation, the most favourable path for **R3** is F, F'' for **S3**, and F' for **R4**. The pathways F' and F'' have similar barriers for **S4**. The conformations of **3** have lower barriers ($\sim 8 \text{ kcal mol}^{-1}$) than **4** ($\sim 17 \text{ kcal mol}^{-1}$). On directly comparing the free energies of transition states – **f** + H_2CO_3 , **f'** + HBr + H_2CO_3 , and **f''** + HBr – the most favourable path is the base-assisted F'' for **R4**, **S3**, and **S4**. The direct path F is most favorable for **R3**.

All the three routes of C-C formation results in the generation of the product scaffold coordinated with PdL, PdL(H)(Br), or PdL(H_2CO_3). These product-complexes span all the conceivable isomeric product geometries. The **BS3** and **BR4** has the -CH₃ and -OH groups in the opposite sides of the newly formed five membered ring, while they are in the same side in **BR3** and **BS4**. The products are released (G) from these intermediates.

β -hydride elimination in the 6-*endo*-cyclization pathway(M)

All mechanisms discussed so far lead to the product **2** (Figure 1) through a 5-*exo* cyclization followed by other steps. Another possible route is through a 6-*endo* cyclization (D) instead of 5-*exo* cyclization, after the oxidative addition (C). This pathway leads to the product **g-6** after the β -hydride elimination (L). The β -hydride elimination is endergonic by $7.74 \text{ kcal mol}^{-1}$ for **BR4** and $7.58 \text{ kcal mol}^{-1}$ for **BS4**. The free energies of activation ($\Delta^\ddagger G^L$) barriers

Figure 12: Reaction profiles for C-H activation process through two pathways: *Top*) direct path (d to f), and *Bottom*) base assisted path (d to f'')

are similar, 8.07 kcal mol⁻¹ (**BR4c**) and 7.46 kcal mol⁻¹ (**BS4c**). The transition states and the intermediates (**1-6**) are nearly isoenergetic. For **BS4c**, the Gibbs free energy of the TS is lower by 0.12 kcal mol⁻¹ than the intermediates due to higher entropy, but the total energy (*E*) of the TS is higher by 0.44 kcal mol⁻¹.

Conclusion

We have studied all the steps in the catalytic cycle of *tandem* Heck reaction/C-H activation reaction, **1** → **2** (Figure 1) using the Density Functional Theory based calculations. We analyzed the pathways for the formation of two possible products and many possible pathways. This study consider many conformations of the substrate for the large part of the catalytic cycle.

To account for the conformational flexibility of the substrate, a series of steps based on i) a molecular mechanics (MMFF94) based conformational search using RDKit, ii) clustering of the RI-BP86-D3BJ/def2-SVP optimized geometries, and iii) modeling and optimization of enantiomer used. Eight different conformations selected this way were used for the analysis of catalytic cycle.

The coordination of PdL to *re* and *si* faces of the substrates produce 16 π -complexes with the complexation energies ranging between 30-43 kcal mol⁻¹. The complexes where one of the double bond is coordinated (**MXn**) is less stable than the bidentate complexes with coordination from both the double bonds (**BXn**). The **MXn**'s are more reactive with lower activation energies for oxidative addition compared to **BXn**'s. But the **BXn** transition states for oxidative addition are more stable.

Migratory insertion is the regioselective step. The unique geometries features of the intermediates after the oxidative addition and coordination of the second C=C bond, **Xnc**, has a crucial role in determining the course of migratory insertion. The *twisted* orientation

facilitate 5-*exo* and 6-*endo* cyclization during the migratory insertion, whereas the *eclipsed* orientation allows only 5-*exo* cyclization. The barriers show that the 5-*exo* cyclization is far more favourable, in agreement with the experiments.

The next step in 5-*exo* pathways is the C-H activation where *ortho*-H of phenyl group moves to Pd. This may happen directly or after the exchange of Br⁻ with HCO₃⁻. Among the four conformations analyzed, the latter pathway has lower activation free energies for three of them. The other way to compare the path is to compare the energies of the transition states. In this way, the former direct pathway is more favourable for three conformations.

The next important step is the second C-C bond formation. Here also we analyzed three pathways. Comparing these pathways on stepwise barriers, each of the conformations have different favourable pathways. But on comparing the energies of the transition states, the most favourable path is the base-assisted pathway for three conformations.

Conflicts of interest

The authors declare no conflict of interests

Acknowledgements

We thank computational facilities from DST FIST grants (SR/FST/CSII-026/2013 and SR/FST/CSII-011/2005). DYR thank UGC for fellowship.

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Computational Study of *Tandem* C-C Coupling
and C-H Activation Reaction of a Flexible
Substrate

Davuluri Yogeswara Rao, Anakuthil Anoop*

Supporting Information

Figure 1: NCI-plot for substrates

Figure 2: Reaction Profile for C-H activation process by base assist mechanism(d to f')

Figure 3: Reaction Profile for C-H activation process by HBr elimination mechanism(d to f')

Figure 4: Reaction Profile for C-H activation process in BR3 path

Figure 5: Reaction Profile for C-H activation process in BR4 path

Figure 6: Reaction Profile for C-H activation process in BS3 path

Figure 7: Reaction Profile for C-H activation process in BS4 path

Figure 8: Reaction Profile of complete catalytic cycle (1+PdPPh₃, A, B, C, D(exo), E, F, X, and g+PPh₃Pd(H)Br) for R3, R4, S3, and S4

Cartesian coordinates

Optimized Substrate Geometries(Xn)

```
R1
40
SCF Energy = -3384.324630463
C      0.1641519      3.8596021     -2.6943423
C     -0.4793661      3.8600671     -1.4352201
C     -1.8912192      3.8318333     -1.3930792
C     -2.6387050      3.7727622     -2.5775052
C     -1.9892860      3.7566998     -3.8233897
C     -0.5858776      3.8066351     -3.8761968
C      0.3280151      3.8752638     -0.1941455
C      1.3904422      3.0778083      0.1028056
C      1.7513999      1.9720853     -0.8333983
C      0.7836993      1.0215640     -1.2336978
C      1.1094655     -0.0083205     -2.1244640
C      2.4119245     -0.1095417     -2.6419141
C      3.3804911      0.8335950     -2.2633209
C      3.0578720      1.8653378     -1.3681604
Br     -0.2445710      5.2259051      1.0740407
C      1.3485381      1.1180836      2.4830670
C     -0.0309632      0.6573982      2.0914425
C      2.3785148      0.2584178      2.6622365
C      1.5352102      2.6104435      2.6390008
C      2.2164413      3.2524038      1.3920922
O      3.5430539      2.7871887      1.2616967
H      2.2929380      4.3416467      1.5895058
H      0.5653210      3.1156756      2.8175848
H      2.1985841      2.8400688      3.4975708
H      3.3572996      0.6042431      3.0321331
H      2.2607921     -0.8231180      2.4900132
H     -0.4448638      1.2841321      1.2762921
H     -0.7241461      0.7780416      2.9529759
H     -0.0503795     -0.4029256      1.7748949
H      3.4877952      1.8060405      1.2317946
H     -0.2413424      1.1035538     -0.8477842
H      0.3384499     -0.7361556     -2.4194176
H      2.6687674     -0.9179023     -3.3432226
H      4.3997599      0.7728037     -2.6746040
H      3.8126379      2.6095064     -1.0844745
H     -2.3991865      3.8533944     -0.4174667
H     -3.7376483      3.7407656     -2.5270163
```


H	-2.5768882	3.7141620	-4.7529011
H	-0.0690934	3.8089275	-4.8477572
H	1.2614712	3.8963074	-2.7360684

R2
40

SCF Energy = -3384.324152143

C	0.0730715	3.7876234	-2.6634649
C	-0.5563034	3.7700971	-1.3974210
C	-1.9629395	3.6512945	-1.3394788
C	-2.7164376	3.5228488	-2.5143226
C	-2.0798888	3.5256185	-3.7670486
C	-0.6833994	3.6641967	-3.8361983
C	0.2601932	3.8553427	-0.1653707
C	1.3745508	3.1312160	0.1202012
C	1.7875576	2.0339571	-0.8022363
C	0.8950429	0.9771634	-1.0929696
C	1.2811690	-0.0721944	-1.9355405
C	2.5672480	-0.0880709	-2.5040070
C	3.4606656	0.9589330	-2.2282317
C	3.0773337	2.0139116	-1.3834754
Br	-0.3976235	5.1563823	1.1109276
C	1.1534386	1.0846337	2.3229915
C	2.2914954	0.1181857	2.0963834
C	-0.1350794	0.6848878	2.2730204
C	1.5008520	2.5317435	2.5926649
C	2.1711725	3.3045822	1.4204453
O	3.5506035	3.0000738	1.2826475
H	2.1427346	4.3801186	1.6898766
H	0.5802011	3.0808662	2.8727829
H	2.2070649	2.6076175	3.4489526
H	-0.9599122	1.3985791	2.4258785
H	-0.4044392	-0.3654266	2.0773793
H	3.0730024	0.2189909	2.8785215
H	2.7826111	0.2972709	1.1130227
H	1.9413736	-0.9319863	2.0811883
H	3.6248463	2.0558110	1.0430240
H	-0.1036380	0.9870903	-0.6358567
H	0.5733809	-0.8875038	-2.1490553
H	2.8701841	-0.9145151	-3.1646404
H	4.4646083	0.9615281	-2.6795359
H	3.7687613	2.8428522	-1.1799220
H	-2.4611222	3.6557834	-0.3588034
H	-3.8104369	3.4207554	-2.4510542
H	-2.6728128	3.4284953	-4.6890710
H	-0.1773238	3.6820610	-4.8132485

H	1.1647939	3.8977858	-2.7186554
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R3

40

SCF Energy = -3384.321867227

C	0.0944895	3.7664430	-2.6750965
C	-0.5579408	3.7847326	-1.4211781
C	-1.9660148	3.6705831	-1.3857285
C	-2.6982451	3.5107801	-2.5700896
C	-2.0388757	3.4795861	-3.8105765
C	-0.6412360	3.6144417	-3.8579343
C	0.2321647	3.8918916	-0.1726593
C	1.3177058	3.1411163	0.1507657
C	1.7455395	2.0353324	-0.7581960
C	0.8939972	0.9321460	-0.9894798
C	1.2942708	-0.1178479	-1.8270310
C	2.5546560	-0.0867101	-2.4476979
C	3.4097817	1.0048540	-2.2275819
C	3.0115882	2.0592056	-1.3894974
Br	-0.4536179	5.2059445	1.0691155
C	0.3662480	2.2302161	3.0866175
C	-0.7645994	1.5830657	2.3277231
C	0.1667109	2.8511440	4.2678682
C	1.7542500	2.1657375	2.4784403
C	2.1040837	3.2786475	1.4541425
O	3.5089986	3.3004640	1.2195487
H	1.8632039	4.2602743	1.9062582
H	2.5171007	2.2585269	3.2777317
H	1.9126196	1.1801096	1.9836684
H	0.9991935	3.3147592	4.8210791
H	-0.8367910	2.9247530	4.7158655
H	-0.5414382	0.5141116	2.1207769
H	-0.9167540	2.0712808	1.3429732
H	-1.7178405	1.6394229	2.8870913
H	3.7630802	2.4050563	0.9173970
H	-0.0951189	0.9117986	-0.5111576
H	0.6151491	-0.9667582	-1.9984643
H	2.8670692	-0.9103069	-3.1073237
H	4.3925993	1.0444121	-2.7216737
H	3.6639956	2.9316411	-1.2429111
H	-2.4824034	3.7064346	-0.4150457
H	-3.7934228	3.4126014	-2.5240228
H	-2.6151112	3.3593927	-4.7404218
H	-0.1175590	3.6063286	-4.8257783
H	1.1868731	3.8742874	-2.7141171

```

R4
40
SCF Energy = -3384.323553539
C      0.2120622      3.9021169      -2.7155913
C     -0.4610486      3.9128342      -1.4730441
C     -1.8724498      3.8508872      -1.4614693
C     -2.5899889      3.7524540      -2.6613534
C     -1.9112382      3.7296646      -3.8918358
C     -0.5088748      3.8102604      -3.9138784
C      0.3105813      3.9580401      -0.2092624
C      1.3448882      3.1432395       0.1223140
C      1.7126543      2.0216807      -0.7923625
C      0.7753360      1.0062086      -1.0869813
C      1.1159869     -0.0603753      -1.9294544
C      2.4016861     -0.1340723      -2.4925417
C      3.3410529      0.8706121      -2.2113444
C      3.0024599      1.9419712      -1.3682793
Br    -0.2976450      5.3303414       1.0098006
C      0.1867391      2.2861927       2.9188965
C      0.0069592      3.2770807       4.0410422
C     -0.8474563      1.6080671       2.3795840
C      1.6006322      2.0986324       2.4166317
C      2.1016585      3.2064281       1.4482210
O      3.5109257      3.1116209       1.2767077
H      1.9278676      4.2019192       1.9013077
H      2.3153491      2.0952799       3.2675482
H      1.6984921      1.1214850       1.8958724
H     -0.6902298      0.8693373       1.5784660
H     -1.8810992      1.7642379       2.7261887
H      0.4307335      4.2680128       3.7743621
H      0.5434777      2.9357018       4.9530917
H     -1.0598059      3.4215658       4.2979926
H      3.7009884      2.2021497       0.9695635
H     -0.2339853      1.0747296      -0.6567296
H      0.3708525     -0.8395658      -2.1506504
H      2.6681930     -0.9709605      -3.1556101
H      4.3447241      0.8291777      -2.6614730
H      3.7238174      2.7487415      -1.1759141
H     -2.4007031      3.8738496      -0.4968899
H     -3.6887047      3.6937337      -2.6357893
H     -2.4760265      3.6567799      -4.8335672
H      0.0300842      3.8060875      -4.8733494
H      1.3087539      3.9656522      -2.7326192

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S1
40

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```

SCF Energy = -3384.321343614
C      0.0357325      3.7618557      -2.6233111
C     -0.5718494      3.6905107      -1.3485636
C     -1.9682511      3.4914840      -1.2687032
C     -2.7325034      3.3357947      -2.4333409
C     -2.1171981      3.3916049      -3.6954196
C     -0.7319983      3.6110674      -3.7850817
C      0.2615382      3.8045827      -0.1322275
C      1.4166669      3.1416668       0.1371300
C      1.8626223      2.0538381      -0.7788961
C      0.9890562      1.0122242      -1.1633865
C      1.4272324     -0.0110808      -2.0126239
C      2.7449993     -0.0106353      -2.5017285
C      3.6229709      1.0199746      -2.1277105
C      3.1886168      2.0395419      -1.2679848
Br    -0.4463582      5.1048166      1.1390943
C      1.3395007      1.3089393      2.4817307
C     -0.1298382      1.0347508      2.2889130
C      2.2671024      0.3298086      2.4618721
C      1.7365075      2.7635718      2.6563313
C      2.3195772      3.3903263      1.3588281
O      2.7044624      4.7382334      1.5316529
H      3.2627751      2.8467831      1.1499074
H      0.8632349      3.3663658      2.9788032
H      2.5181257      2.8770634      3.4348035
H      3.3367081      0.5476767      2.6135202
H      1.9909838     -0.7215089      2.2854728
H     -0.5428807      1.6531711      1.4638206
H     -0.7027063      1.3170588      3.1991041
H     -0.3306216     -0.0309679      2.0666283
H      1.8837435      5.2519642      1.6872941
H     -0.0412635      1.0079815     -0.7820559
H      0.7343672     -0.8186652     -2.2935377
H      3.0878549     -0.8142501     -3.1707995
H      4.6554655      1.0318959     -2.5087637
H      3.8774576      2.8513293     -0.9886383
H     -2.4510735      3.4541836     -0.2807511
H     -3.8176653      3.1704008     -2.3547675
H     -2.7187083      3.2729214     -4.6092592
H     -0.2444378      3.6702934     -4.7698062
H      1.1193516      3.9312267     -2.6916495

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S2
40
SCF Energy = -3384.323765635
C      0.0394431      3.8325224     -2.6596784

```

C	-0.5805059	3.7453379	-1.3918910
C	-1.9808352	3.5692860	-1.3287761
C	-2.7370019	3.4527398	-2.5030977
C	-2.1096100	3.5241685	-3.7585169
C	-0.7199785	3.7196326	-3.8313353
C	0.2436717	3.8190761	-0.1660401
C	1.3858532	3.1320071	0.0922459
C	1.8090026	2.0501503	-0.8419192
C	0.9198132	1.0143619	-1.2042298
C	1.3362534	-0.0168900	-2.0551096
C	2.6475938	-0.0321148	-2.5619764
C	3.5418031	0.9909840	-2.2061072
C	3.1286899	2.0204679	-1.3466865
Br	-0.4584357	5.0939721	1.1330630
C	1.2222004	1.1572626	2.3102643
C	2.3367310	0.1678922	2.0807574
C	-0.0790874	0.8019950	2.2575611
C	1.6248804	2.5923097	2.5641676
C	2.2712737	3.2991098	1.3376990
O	2.6548860	4.6266016	1.6258222
H	3.2219600	2.7756630	1.1109742
H	0.7386909	3.1819295	2.8727095
H	2.3695046	2.6550851	3.3873831
H	-0.8795431	1.5422317	2.4147273
H	-0.3830815	-0.2372845	2.0545683
H	3.0547209	0.1724182	2.9289943
H	2.9186291	0.4241115	1.1692731
H	1.9523330	-0.8618354	1.9512351
H	1.8317848	5.1288578	1.8052905
H	-0.0981394	1.0203219	-0.7910919
H	0.6328557	-0.8204576	-2.3211021
H	2.9735114	-0.8436259	-3.2300276
H	4.5694166	0.9889311	-2.6002521
H	3.8291043	2.8264870	-1.0787495
H	-2.4724704	3.5168111	-0.3460236
H	-3.8255700	3.3048600	-2.4374366
H	-2.7049428	3.4360588	-4.6798498
H	-0.2223110	3.7905708	-4.8102492
H	1.1262062	3.9854933	-2.7151893

S3

40

SCF Energy = -3384.321804377

C	0.0689516	3.8254595	-2.7153852
C	-0.5981952	3.8183095	-1.4691640
C	-1.9982082	3.6294080	-1.4488626

C	-2.7064506	3.4201708	-2.6402105
C	-2.0312804	3.4126411	-3.8725841
C	-0.6422401	3.6222238	-3.9051339
C	0.1768109	3.9872913	-0.2168117
C	1.2999727	3.2968601	0.1157316
C	1.7040071	2.1379122	-0.7369797
C	0.7999870	1.0806067	-0.9860173
C	1.1780206	-0.0162124	-1.7710845
C	2.4688714	-0.0792463	-2.3232536
C	3.3797335	0.9611460	-2.0775670
C	3.0032880	2.0569491	-1.2862023
Br	-0.6106726	5.3118312	0.9617394
C	0.6528970	2.6365427	3.1691724
C	-0.5698152	1.9388391	2.6307492
C	0.5999851	3.4644897	4.2371548
C	1.9553181	2.4206995	2.4300707
C	2.2175328	3.5016768	1.3307745
O	2.2754504	4.7973067	1.8605382
H	3.2418929	3.2980638	0.9508754
H	2.8076947	2.4829482	3.1356222
H	1.9819304	1.4180435	1.9551106
H	1.5077778	3.9462033	4.6336841
H	-0.3486540	3.6691758	4.7583872
H	-0.4233241	0.8371765	2.6339418
H	-0.7581870	2.2281366	1.5761676
H	-1.4754412	2.1749823	3.2212889
H	1.4268758	4.9561622	2.3277749
H	-0.2113315	1.1313809	-0.5580284
H	0.4588662	-0.8290567	-1.9535487
H	2.7648884	-0.9391135	-2.9428866
H	4.3911521	0.9232350	-2.5099641
H	3.7173603	2.8776701	-1.1178286
H	-2.5275047	3.6435312	-0.4845491
H	-3.7951801	3.2628819	-2.6061004
H	-2.5888802	3.2525548	-4.8077577
H	-0.1072694	3.6328666	-4.8667569
H	1.1551697	3.9893523	-2.7401062

S4

40

SCF Energy = -3384.320789836

C	0.0802156	3.8154798	-2.6531116
C	-0.5386066	3.8057451	-1.3827714
C	-1.9305189	3.5786960	-1.3028236
C	-2.6790537	3.3383628	-2.4631486
C	-2.0524003	3.3346622	-3.7211341

C	-0.6716897	3.5787879	-3.8114342
C	0.2760305	4.0095590	-0.1625766
C	1.4156206	3.3446523	0.1613112
C	1.8118582	2.1743398	-0.6804866
C	0.9036624	1.1193643	-0.9227457
C	1.2786523	0.0159929	-1.7001665
C	2.5689118	-0.0540832	-2.2527621
C	3.4828126	0.9857130	-2.0153640
C	3.1102793	2.0873403	-1.2302955
Br	-0.4663314	5.4009599	0.9796834
C	0.5685243	2.7234177	3.0997080
C	0.4497868	3.7590485	4.1895748
C	-0.4872113	2.0032030	2.6644987
C	1.9438769	2.5372023	2.5010185
C	2.3232109	3.5586817	1.3765589
O	2.4803414	4.8828870	1.8312720
H	3.3383316	3.2500602	1.0463177
H	2.7243043	2.6371561	3.2846842
H	2.0364980	1.5214550	2.0648842
H	-0.3704393	1.2324156	1.8868296
H	-1.4979192	2.1585448	3.0738003
H	0.9061106	4.7186436	3.8731500
H	1.0155896	3.4369962	5.0913015
H	-0.6018449	3.9393904	4.4841643
H	1.5956222	5.3074975	1.8491845
H	-0.1078552	1.1790642	-0.4968892
H	0.5575743	-0.7966264	-1.8757483
H	2.8626341	-0.9195580	-2.8656658
H	4.4939087	0.9419699	-2.4479165
H	3.8267299	2.9064539	-1.0641744
H	-2.4190939	3.5824294	-0.3171127
H	-3.7607851	3.1515292	-2.3847470
H	-2.6419413	3.1489328	-4.6316316
H	-0.1753046	3.5896097	-4.7935009
H	1.1606088	4.0050235	-2.7211346

Catalyst

Pd-PPh3

35

SCF Energy = -1163.896646601

Pd	0.0014905	-0.0069045	0.3903040
P	0.0006561	-0.0032558	2.5559726
C	1.6577943	0.1152833	3.3623163

C	-0.9293459	1.3756807	3.3585243
C	-0.7278530	-1.4956092	3.3637236
C	1.8917176	0.8978056	4.5110888
C	3.1681654	0.9220924	5.0980853
C	4.2137238	0.1618046	4.5498492
C	3.9836175	-0.6207764	3.4038480
C	2.7150921	-0.6369513	2.8074890
H	1.0733741	1.4896176	4.9470021
H	3.3448833	1.5402798	5.9916490
H	5.2127362	0.1838455	5.0113272
H	4.8018619	-1.2127849	2.9661292
H	2.5281324	-1.2263022	1.8950282
C	-1.7334824	1.1894043	4.5009768
C	-2.3906406	2.2854259	5.0852805
C	-2.2435862	3.5712864	4.5406372
C	-1.4414350	3.7608148	3.4007542
C	-0.7951853	2.6677756	2.8070341
H	-1.8461729	0.1845790	4.9340894
H	-3.0217077	2.1313001	5.9740256
H	-2.7603936	4.4275741	5.0001502
H	-1.3286151	4.7656770	2.9658721
H	-0.1836000	2.7988786	1.8995371
C	-0.1648235	-2.0936480	4.5091909
C	-0.7846990	-3.2091292	5.0974892
C	-1.9708827	-3.7281416	4.5539545
C	-2.5358037	-3.1335313	3.4110712
C	-1.9128939	-2.0290984	2.8133257
H	0.7607999	-1.6859284	4.9413877
H	-0.3358952	-3.6745375	5.9884457
H	-2.4535587	-4.6024109	5.0166932
H	-3.4616595	-3.5409700	2.9770846
H	-2.3317600	-1.5691458	1.9034888

Optimized Geometries(BXna)

R1
75
SCF Energy = -4548.306560953

C	2.5130515	1.1784604	-2.3455717
C	1.5879454	1.5168222	-1.3280432
C	0.4369107	2.2530947	-1.7156954
C	0.1870472	2.5725413	-3.0517763
C	1.0896945	2.1831225	-4.0585269
C	2.2560381	1.4984396	-3.6902204

C	1.7252891	1.0980053	0.1021446
C	2.5000569	0.0339998	0.6750709
C	3.3573483	-0.7899594	-0.2476563
C	2.8293965	-1.8475975	-1.0157623
C	3.6430437	-2.5694417	-1.9008310
C	5.0102367	-2.2646671	-2.0144158
C	5.5574318	-1.2299439	-1.2373517
C	4.7372297	-0.4950033	-0.3651142
Br	1.2996832	2.6166951	1.3089286
C	0.6966314	-1.1563226	2.8011533
C	-0.6189252	-0.9188852	3.5085494
C	0.9279626	-2.3377424	2.1118355
C	1.7994336	-0.1633069	3.1670635
C	2.9620679	-0.0292221	2.1698984
O	3.8005793	-1.1552569	2.4060573
H	3.5068144	0.9202116	2.4095057
H	1.3360283	0.8303060	3.3112072
H	2.2389529	-0.4500053	4.1496183
H	1.9487145	-2.6277352	1.8253593
H	0.1322651	-3.0955351	2.0505041
H	-0.9880262	0.1129333	3.3357499
H	-0.4815124	-1.0292113	4.6075526
H	-1.3999455	-1.6307688	3.1806715
H	4.4390456	-1.2185748	1.6669927
H	1.7561356	-2.0826175	-0.9143468
H	3.2054765	-3.3798028	-2.5033658
H	5.6497715	-2.8342530	-2.7053979
H	6.6261271	-0.9805852	-1.3222675
H	5.1583697	0.3535951	0.1980701
H	-0.2854911	2.5507418	-0.9458051
H	-0.7326747	3.1199950	-3.3067252
H	0.8902288	2.4233638	-5.1135923
H	2.9939214	1.2099769	-4.4547380
H	3.4431459	0.6583509	-2.1001621
Pd	0.4525849	-0.5817030	0.6039883
P	-1.6814500	-0.5388674	-0.2245870
C	-2.4429216	1.1304542	-0.3449170
C	-2.2969187	1.9909031	0.7648468
H	-1.7744824	1.6296623	1.6636933
C	-2.7673980	3.3097725	0.7050000
H	-2.6387601	3.9753982	1.5716169
C	-3.3726768	3.7877189	-0.4708590
H	-3.7244499	4.8290788	-0.5256473
C	-3.5178187	2.9361812	-1.5787774
H	-3.9866503	3.3084447	-2.5025585
C	-3.0592652	1.6101476	-1.5174967

H	-3.1598266	0.9499372	-2.3913044
C	-1.7313514	-1.1629522	-1.9560124
C	-2.8499687	-1.8321074	-2.4940314
H	-3.7303116	-2.0211786	-1.8613191
C	-2.8371895	-2.2578535	-3.8321958
H	-3.7117729	-2.7826389	-4.2464403
C	-1.7134964	-2.0140589	-4.6409880
H	-1.7081985	-2.3480944	-5.6898705
C	-0.5970288	-1.3476502	-4.1075753
H	0.2876923	-1.1489029	-4.7305266
C	-0.6012119	-0.9292644	-2.7690794
H	0.2731962	-0.4099024	-2.3503439
C	-2.9722984	-1.5415043	0.6224178
C	-2.6744555	-2.9022959	0.8593896
H	-1.7227851	-3.3174193	0.4904291
C	-3.5776007	-3.7153422	1.5570554
H	-3.3389631	-4.7757584	1.7305847
C	-4.7815827	-3.1734959	2.0440567
H	-5.4862166	-3.8084122	2.6021926
C	-5.0794867	-1.8204713	1.8172284
H	-6.0208024	-1.3925401	2.1948489
C	-4.1824612	-1.0062626	1.1041782
H	-4.4211325	0.0522031	0.9226674

R2

75

SCF Energy = -4548.309140807

C	1.7114328	1.9703644	-1.9918753
C	1.0407422	1.9087080	-0.7438095
C	-0.1183367	2.7118151	-0.5978610
C	-0.6158886	3.4907713	-1.6477786
C	0.0445630	3.5151614	-2.8883707
C	1.2177682	2.7607774	-3.0408626
C	1.5044784	1.0577908	0.3941694
C	2.5111371	0.0499031	0.4356373
C	3.0968283	-0.4272620	-0.8651589
C	2.3625646	-1.2573736	-1.7399397
C	2.8829553	-1.6387560	-2.9838757
C	4.1606045	-1.2072476	-3.3754668
C	4.9121837	-0.3953091	-2.5088008
C	4.3893901	-0.0074929	-1.2653498
Br	1.1504506	1.9420460	2.1473606
C	1.8176355	-2.2515941	1.9048271
C	2.5827495	-3.2477659	1.0552165
C	0.4825238	-2.5152699	2.2463571
C	2.6443741	-1.2210835	2.6695492

C	3.3791277	-0.2374542	1.7253094
O	4.6933044	-0.6753484	1.4189164
H	3.5257734	0.7253494	2.2552562
H	1.9701715	-0.6414291	3.3302506
H	3.4066213	-1.7072399	3.3213977
H	0.0293588	-2.0363157	3.1301116
H	-0.0128845	-3.4294496	1.8829924
H	3.2424194	-3.8665481	1.7035374
H	3.2235064	-2.7677662	0.2885842
H	1.8977654	-3.9285342	0.5132769
H	4.6226122	-1.4856023	0.8780329
H	1.3578573	-1.5871280	-1.4293904
H	2.2764476	-2.2717386	-3.6472720
H	4.5719675	-1.5037095	-4.3524460
H	5.9136365	-0.0487837	-2.8067389
H	4.9721570	0.6442321	-0.6025362
H	-0.6432184	2.7186550	0.3627664
H	-1.5326902	4.0774735	-1.4881902
H	-0.3421451	4.1256715	-3.7181763
H	1.7712741	2.7825106	-3.9920786
H	2.6325552	1.4066349	-2.1562936
Pd	0.5049263	-0.8612515	0.7644273
P	-1.5936653	-0.7748629	-0.1863214
C	-2.8783373	-2.0381500	0.2337243
C	-2.6475920	0.7352270	-0.1106128
C	-1.2576359	-1.0698016	-1.9665204
C	-3.8588610	-2.4535867	-0.6917889
C	-4.8563121	-3.3601538	-0.3037418
C	-4.8933350	-3.8494201	1.0140851
C	-3.9286975	-3.4277729	1.9431746
C	-2.9225182	-2.5290819	1.5527748
H	-3.8391727	-2.0679155	-1.7222062
H	-5.6140719	-3.6837872	-1.0337011
H	-5.6779250	-4.5596940	1.3162858
H	-3.9554264	-3.8038350	2.9772621
H	-2.1608043	-2.1954935	2.2718778
C	-3.4638085	1.1768830	-1.1697006
C	-4.2496486	2.3295504	-1.0178399
C	-4.2411477	3.0372037	0.1965083
C	-3.4463943	2.5856042	1.2640836
C	-2.6490414	1.4419189	1.1095167
H	-3.4757116	0.6275653	-2.1224966
H	-4.8742129	2.6779701	-1.8546097
H	-4.8567815	3.9422730	0.3113693
H	-3.4344861	3.1361605	2.2168777
H	-1.9911619	1.1054745	1.9264963

C	-1.1104528	-2.3960265	-2.4340612
C	-0.6691820	-2.6414281	-3.7427564
C	-0.3565760	-1.5691800	-4.5969151
C	-0.4813516	-0.2511214	-4.1298264
C	-0.9267263	0.0011066	-2.8240444
H	-1.3408263	-3.2401042	-1.7665594
H	-0.5662542	-3.6787816	-4.0963685
H	-0.0069158	-1.7627805	-5.6222730
H	-0.2210312	0.5980269	-4.7786789
H	-1.0034139	1.0372771	-2.4692284

R3

75

SCF Energy = -4548.312347916

C	1.6984538	2.0322427	-2.3649320
C	1.3557625	0.8979659	-1.5996090
C	1.2083853	-0.3400153	-2.2640082
C	1.4199797	-0.4480991	-3.6427991
C	1.7634993	0.6874939	-4.3942444
C	1.8982976	1.9278845	-3.7494319
C	1.1842521	0.9689440	-0.1194700
C	2.0712701	0.3273845	0.8023588
C	3.2127992	-0.4488604	0.2092810
C	3.1356765	-1.8271729	-0.0704058
C	4.2260776	-2.5144643	-0.6238389
C	5.4195294	-1.8296147	-0.9072344
C	5.5067808	-0.4522768	-0.6480771
C	4.4114823	0.2347570	-0.0994279
Br	0.2724285	2.6346739	0.4697674
C	1.0619615	-1.4293772	2.9092351
C	1.3956659	-2.9040338	2.8181078
C	-0.2682620	-1.0459694	3.1000836
C	2.2488907	-0.4961007	3.1735832
C	2.2759709	0.7592288	2.2733185
O	3.4493970	1.5362697	2.4809339
H	1.4357645	1.4294897	2.5430709
H	2.2852229	-0.1846384	4.2400102
H	3.1859897	-1.0624352	2.9803808
H	-0.5101015	-0.0480052	3.5041645
H	-1.0540626	-1.8109183	3.1986786
H	2.2152959	-3.1042367	2.1014202
H	0.5138741	-3.5106889	2.5339448
H	1.7502641	-3.2635471	3.8106234
H	4.2079216	0.9591299	2.2581366
H	2.1864218	-2.3446219	0.1326096
H	4.1407452	-3.5899772	-0.8423070

H	6.2756868	-2.3661828	-1.3434944
H	6.4294239	0.0972920	-0.8900301
H	4.4623210	1.3213798	0.0645619
H	0.8906512	-1.2133816	-1.6774050
H	1.2849029	-1.4213116	-4.1369339
H	1.9114832	0.6089225	-5.4820071
H	2.1632263	2.8255907	-4.3289775
H	1.7995196	3.0052821	-1.8624071
Pd	0.1165938	-0.5360865	0.9677509
P	-1.9655185	-0.7222912	-0.0054665
C	-2.0075474	-0.4590643	-1.8262809
C	-1.7525074	0.8471676	-2.3023869
H	-1.5938169	1.6683022	-1.5864442
C	-1.6773847	1.0936826	-3.6779556
H	-1.4654695	2.1116470	-4.0362775
C	-1.8371756	0.0393734	-4.5941937
H	-1.7616239	0.2323157	-5.6748851
C	-2.0823997	-1.2607217	-4.1262324
H	-2.2091160	-2.0898016	-4.8393128
C	-2.1708652	-1.5121780	-2.7461389
H	-2.3672477	-2.5322954	-2.3840436
C	-3.3070420	0.3984616	0.5683593
C	-3.1939215	0.9782688	1.8474122
H	-2.3000144	0.7662600	2.4510249
C	-4.1987972	1.8309913	2.3297111
H	-4.0996868	2.2832911	3.3280930
C	-5.3198869	2.1177262	1.5333237
H	-6.1046328	2.7923295	1.9082662
C	-5.4321669	1.5528454	0.2509667
H	-6.3040972	1.7844342	-0.3796955
C	-4.4295169	0.6985222	-0.2329041
H	-4.5072931	0.2722224	-1.2445220
C	-2.6577507	-2.4187252	0.1926908
C	-4.0329254	-2.6982474	0.3113876
H	-4.7632547	-1.8758331	0.2917616
C	-4.4712014	-4.0238699	0.4670775
H	-5.5470202	-4.2336669	0.5684483
C	-3.5436276	-5.0785294	0.4950561
H	-3.8913552	-6.1156056	0.6171796
C	-2.1694867	-4.8056660	0.3759624
H	-1.4376238	-5.6273452	0.4031958
C	-1.7290599	-3.4813620	0.2365714
H	-0.6529094	-3.2484753	0.1695088

R4
75

SCF Energy = -4548.317163648

C	3.9379688	-0.4285305	-1.3283509
C	2.8711307	-0.7844483	-0.4732299
C	2.2605977	-2.0458165	-0.6390460
C	2.6867903	-2.9208375	-1.6491768
C	3.7416316	-2.5533950	-2.5010889
C	4.3687851	-1.3073879	-2.3347201
C	2.4288596	0.1955040	0.5848327
Pd	0.3968722	-0.1583903	1.1777411
P	-1.6459817	-0.4127529	0.1079239
C	1.6841986	1.3301637	0.1511424
Br	1.5561043	2.8521077	1.4018745
C	1.4152296	1.7102536	-1.2670573
C	1.6022358	3.0280173	-1.7392523
C	1.3134085	3.3692882	-3.0697464
C	0.8400397	2.4005773	-3.9667290
C	0.6686903	1.0811447	-3.5152503
C	0.9445254	0.7435907	-2.1870582
C	3.2902049	0.1135068	1.8726673
O	4.6781233	0.0733826	1.5876948
C	2.7914456	-1.0728671	2.7208020
C	1.3243888	-0.8605242	3.0800949
C	0.3063684	-1.7598597	2.7241228
C	1.0615154	0.1755390	4.1567206
H	3.1377406	1.0532932	2.4377789
H	3.4159910	-1.1615913	3.6369872
H	2.9172296	-2.0114812	2.1397007
H	0.5525744	-2.6993234	2.2022184
H	-0.6615758	-1.7395734	3.2492078
H	1.4587593	-0.1905437	5.1303512
H	-0.0213291	0.3698081	4.2811285
H	1.5565331	1.1427296	3.9430946
H	4.8283929	-0.7059496	1.0141680
H	1.4056697	-2.3105619	0.0005963
H	2.1751307	-3.8862049	-1.7767329
H	4.0717555	-3.2355580	-3.2993339
H	5.1915541	-1.0095007	-3.0023744
H	4.4065824	0.5593886	-1.2117258
H	0.7688022	-0.2815494	-1.8419667
H	0.2962266	0.3053589	-4.2015542
H	0.6004415	2.6705709	-5.0060663
H	1.4583577	4.4083574	-3.4031129
H	1.9635348	3.7997212	-1.0456466
C	-2.2720622	0.8705648	-1.0532775
C	-3.1194908	-0.7798521	1.1539247
C	-1.4577664	-1.9337769	-0.9108637

C	-1.2172216	-1.8935101	-2.2998211
C	-0.8688988	-3.0629684	-2.9948009
C	-0.7663197	-4.2877244	-2.3170583
C	-1.0205120	-4.3393014	-0.9343259
C	-1.3593664	-3.1727014	-0.2356440
H	-1.2956303	-0.9400636	-2.8397163
H	-0.6753280	-3.0127890	-4.0770212
H	-0.4930184	-5.2026291	-2.8641036
H	-0.9505349	-5.2961980	-0.3949038
H	-1.5459111	-3.2162893	0.8478836
C	-3.2526527	0.6150261	-2.0341776
C	-3.6378056	1.6300309	-2.9225593
C	-3.0565803	2.9072920	-2.8292928
C	-2.1026817	3.1736067	-1.8345304
C	-1.7130025	2.1590301	-0.9477474
H	-3.7089954	-0.3832412	-2.1126510
H	-4.3955106	1.4234747	-3.6939250
H	-3.3526314	3.6980933	-3.5353439
H	-1.6438367	4.1698198	-1.7549477
H	-0.9562121	2.3549574	-0.1740553
C	-4.1746620	-1.6157014	0.7349272
C	-5.2788439	-1.8302510	1.5742957
C	-5.3411801	-1.2083136	2.8333870
C	-4.2922867	-0.3741763	3.2556002
C	-3.1823172	-0.1668277	2.4220285
H	-4.1246104	-2.1120576	-0.2460758
H	-6.0970312	-2.4882686	1.2435441
H	-6.2080761	-1.3793328	3.4895646
H	-4.3344799	0.1105901	4.2428006
H	-2.3452719	0.4717752	2.7480129

S1

75

SCF Energy = -4548.311018803

C	2.7343295	1.6797997	-2.3146356
C	1.5696692	1.5953677	-1.5200093
C	0.3400121	2.0126571	-2.0817472
C	0.2677043	2.4598892	-3.4052818
C	1.4271831	2.5010901	-4.2015227
C	2.6578767	2.1160767	-3.6470764
C	1.6076929	1.1048238	-0.1119198
C	2.4693315	0.0967440	0.4344260
C	3.3021240	-0.7050485	-0.5260695
C	2.7202301	-1.4965150	-1.5406958
C	3.5180317	-2.2141011	-2.4421099
C	4.9187886	-2.1598702	-2.3430363

C	5.5106489	-1.3876245	-1.3290785
C	4.7122822	-0.6683744	-0.4263186
Br	1.1277487	2.6432191	1.0978106
C	0.8377351	-1.1801333	2.6657862
C	-0.4433143	-1.0287542	3.4538558
C	1.0793761	-2.3293607	1.9294862
C	1.8979448	-0.1274214	2.9635859
C	2.9942820	0.0570093	1.8916435
O	3.8565994	1.1456705	2.2010478
H	3.6472184	-0.8379720	1.9348993
H	1.3898665	0.8445789	3.1225655
H	2.3950860	-0.3689976	3.9309497
H	2.0730541	-2.5684304	1.5210066
H	0.3266250	-3.1314079	1.9134303
H	-0.8956728	-0.0292260	3.2906328
H	-0.2283266	-1.1086059	4.5426768
H	-1.1906599	-1.7989425	3.1861572
H	3.3205024	1.9557403	2.0560635
H	1.6210401	-1.5457745	-1.6098036
H	3.0401287	-2.8239881	-3.2238639
H	5.5473609	-2.7226895	-3.0497640
H	6.6071264	-1.3385937	-1.2424506
H	5.1743768	-0.0399372	0.3501693
H	-0.5668540	1.9717046	-1.4624551
H	-0.7041204	2.7672824	-3.8202494
H	1.3714916	2.8416043	-5.2467184
H	3.5754289	2.1604329	-4.2535275
H	3.7048950	1.3935595	-1.8898361
Pd	0.4400732	-0.5932475	0.4516287
P	-1.7489011	-0.6819697	-0.2030209
C	-2.6376029	0.9266124	-0.2990195
C	-2.3911832	1.8659588	0.7251115
H	-1.6919269	1.6097603	1.5354025
C	-2.9953116	3.1304421	0.6855164
H	-2.7896202	3.8586325	1.4843423
C	-3.8366581	3.4744212	-0.3866118
H	-4.2973998	4.4730566	-0.4273065
C	-4.0788636	2.5455463	-1.4127075
H	-4.7323892	2.8142725	-2.2567282
C	-3.4865265	1.2730443	-1.3696173
H	-3.6723525	0.5494110	-2.1770672
C	-1.9483476	-1.3819995	-1.8946935
C	-3.0471467	-2.1825574	-2.2688231
H	-3.8215245	-2.4297969	-1.5273739
C	-3.1497961	-2.6657181	-3.5835807
H	-4.0079988	-3.2936090	-3.8682407

C	-2.1637443	-2.3483446	-4.5333782
H	-2.2481072	-2.7292128	-5.5626246
C	-1.0693993	-1.5467344	-4.1655481
H	-0.2929354	-1.2906804	-4.9019695
C	-0.9577994	-1.0710105	-2.8509859
H	-0.1047073	-0.4394676	-2.5618451
C	-2.8682324	-1.7278551	0.8183938
C	-2.5040604	-3.0821053	0.9945952
H	-1.6239203	-3.4784098	0.4634793
C	-3.2530927	-3.9144744	1.8368612
H	-2.9650965	-4.9695333	1.9610902
C	-4.3643081	-3.3992244	2.5299112
H	-4.9458927	-4.0491548	3.2010101
C	-4.7278167	-2.0538710	2.3614611
H	-5.5982159	-1.6466837	2.8984231
C	-3.9882813	-1.2205098	1.5042969
H	-4.2797910	-0.1682693	1.3707013

S2

75

SCF Energy = -4548.314520697

C	2.2465450	2.4120246	-1.9710228
C	1.6761574	1.2360421	-1.4399272
C	1.1927231	0.2602156	-2.3383132
C	1.2847522	0.4468723	-3.7222329
C	1.8477508	1.6243560	-4.2395786
C	2.3279726	2.6059946	-3.3574543
C	1.6192057	0.9948100	0.0317991
C	2.4512192	0.0626253	0.7241482
C	3.2789197	-0.8307536	-0.1580739
C	2.7828123	-2.0308782	-0.7010144
C	3.5839329	-2.8288061	-1.5323166
C	4.8988704	-2.4352606	-1.8277300
C	5.4083787	-1.2448901	-1.2799854
C	4.6070554	-0.4492303	-0.4483106
Br	1.1226383	2.6729323	1.0368194
C	1.1561163	-1.2540703	2.8570783
C	1.8826362	-2.5784619	2.7188060
C	-0.2440005	-1.2326795	2.9475798
C	2.0091718	-0.0504407	3.2536251
C	3.0614829	0.2369262	2.1574459
O	3.7793262	1.4421767	2.3327151
H	3.8352900	-0.5543692	2.2257206
H	1.3651495	0.8428875	3.3850772
H	2.5305221	-0.2286347	4.2221671
H	-0.7700199	-0.3726129	3.3928678

H	-0.8065494	-2.1793100	2.9028423
H	2.2771677	-2.8918300	3.7114519
H	2.7445810	-2.5312848	2.0260039
H	1.2032401	-3.3746390	2.3571909
H	3.1339710	2.1682626	2.1869680
H	1.7491441	-2.3227611	-0.4570170
H	3.1776002	-3.7617167	-1.9520544
H	5.5283565	-3.0561956	-2.4831163
H	6.4384237	-0.9302087	-1.5076308
H	4.9973642	0.4848738	-0.0164203
H	0.7146158	-0.6385441	-1.9281015
H	0.8873579	-0.3234715	-4.3991152
H	1.9030701	1.7813360	-5.3274424
H	2.7726657	3.5329235	-3.7508001
H	2.6197988	3.1849477	-1.2835854
Pd	0.3366795	-0.4159455	0.9552479
P	-1.7565327	-0.2437720	-0.0310273
C	-1.8697433	0.6606139	-1.6297920
C	-1.3666593	1.9804102	-1.6720927
H	-0.9689700	2.4435426	-0.7563129
C	-1.3310959	2.6884116	-2.8798712
H	-0.9221801	3.7091883	-2.8987587
C	-1.7749618	2.0798115	-4.0657582
H	-1.7246613	2.6273497	-5.0188382
C	-2.2666940	0.7656027	-4.0328622
H	-2.6096933	0.2813101	-4.9599782
C	-2.3186311	0.0573313	-2.8209737
H	-2.6966805	-0.9749599	-2.8064992
C	-2.4215065	-1.9121352	-0.4343923
C	-3.7967084	-2.1474158	-0.6405826
H	-4.5131035	-1.3180938	-0.5388533
C	-4.2480102	-3.4353608	-0.9676578
H	-5.3226079	-3.6146199	-1.1248037
C	-3.3319892	-4.4949270	-1.0929627
H	-3.6899528	-5.5041829	-1.3473491
C	-1.9613268	-4.2662655	-0.8857389
H	-1.2420495	-5.0943806	-0.9753096
C	-1.5092778	-2.9797626	-0.5531233
H	-0.4406036	-2.7828563	-0.3658413
C	-3.1182171	0.4817906	0.9794539
C	-3.4844206	-0.1966214	2.1638129
H	-2.9945276	-1.1476640	2.4189944
C	-4.4790214	0.3246845	3.0020086
H	-4.7600979	-0.2179649	3.9174962
C	-5.1132644	1.5369096	2.6764588
H	-5.8900049	1.9494861	3.3379294

C	-4.7535618	2.2146984	1.5013465
H	-5.2507910	3.1598716	1.2347202
C	-3.7641488	1.6899352	0.6525740
H	-3.5000207	2.2208077	-0.2732424

S3

75

SCF Energy = -4548.311549220

C	2.5533822	0.8889044	-2.8135050
C	1.7557431	0.2377579	-1.8475666
C	1.2362972	-1.0369041	-2.1527786
C	1.5069305	-1.6515653	-3.3827903
C	2.2985510	-0.9938445	-4.3362778
C	2.8230595	0.2783719	-4.0457760
C	1.4846256	0.8608479	-0.5148853
C	2.3058091	0.6211613	0.6416231
C	3.4856416	-0.2859087	0.4304832
C	3.3444630	-1.6646622	0.1664694
C	4.4627780	-2.4724312	-0.0836054
C	5.7531500	-1.9183025	-0.0631236
C	5.9109338	-0.5479000	0.1997328
C	4.7885425	0.2601445	0.4389140
Br	0.7424390	2.7264802	-0.8164354
C	1.3112865	-0.6029370	3.0124577
C	1.8041464	-2.0260827	3.1741299
C	-0.0552031	-0.3381145	3.1461478
C	2.4086133	0.4779684	3.1178802
C	2.3975764	1.4734784	1.9459222
O	1.3089457	2.3509995	2.1794919
H	3.3543597	2.0570533	1.9419620
H	2.3109909	1.0512368	4.0644912
H	3.3949541	-0.0248717	3.1442738
H	-0.4133718	0.6780105	3.3681941
H	-0.7537731	-1.1635166	3.3561506
H	2.6461486	-2.2557616	2.4928687
H	0.9948927	-2.7637374	3.0070467
H	2.1837347	-2.1681211	4.2112184
H	1.1419085	2.8531030	1.3491122
H	2.3324376	-2.0937662	0.1614774
H	4.3237728	-3.5439204	-0.2934481
H	6.6326902	-2.5513615	-0.2549545
H	6.9161952	-0.0992684	0.2083123
H	4.9252599	1.3373900	0.6162018
H	0.6009247	-1.5311367	-1.4038474
H	1.0782197	-2.6408882	-3.6001810
H	2.5050804	-1.4677828	-5.3080744

H	3.4499820	0.7986135	-4.7860893
H	2.9580388	1.8872684	-2.5902800
Pd	0.3498993	-0.1666283	0.9502752
P	-1.8050647	-0.3189658	0.1594983
C	-1.9817129	-0.6759615	-1.6382562
C	-1.6101672	0.3377690	-2.5498493
H	-1.3226834	1.3315200	-2.1744551
C	-1.5765644	0.0736429	-3.9244800
H	-1.2717734	0.8680354	-4.6218567
C	-1.9009584	-1.2058227	-4.4070648
H	-1.8605979	-1.4157225	-5.4865049
C	-2.2714808	-2.2164481	-3.5055342
H	-2.5333487	-3.2191570	-3.8770110
C	-2.3152682	-1.9549738	-2.1254375
H	-2.6081822	-2.7509752	-1.4246692
C	-2.7599764	1.2376553	0.3520836
C	-2.2617517	2.2158275	1.2365284
H	-1.3066734	2.0353925	1.7536644
C	-2.9548423	3.4237060	1.4122613
H	-2.5559260	4.1855744	2.0988882
C	-4.1418648	3.6646947	0.7012352
H	-4.6817297	4.6145429	0.8353846
C	-4.6326377	2.6993836	-0.1958852
H	-5.5542655	2.8932673	-0.7656397
C	-3.9431479	1.4905236	-0.3745997
H	-4.3118849	0.7452509	-1.0958318
C	-2.8195683	-1.6304200	0.9606706
C	-4.1816341	-1.4877775	1.2883886
H	-4.7046794	-0.5468009	1.0637317
C	-4.8689483	-2.5398360	1.9162989
H	-5.9309921	-2.4165551	2.1780364
C	-4.2071436	-3.7429626	2.2117529
H	-4.7496450	-4.5647465	2.7033012
C	-2.8466412	-3.8903773	1.8893609
H	-2.3199071	-4.8270622	2.1272903
C	-2.1536886	-2.8346351	1.2791009
H	-1.0782004	-2.9257191	1.0529615

S4

75

SCF Energy = -4548.309813955

C	3.4156585	1.0632876	-2.2920271
C	2.2200587	0.5026587	-1.7914643
C	1.5624757	-0.4860389	-2.5484558
C	2.0873797	-0.9130226	-3.7782432
C	3.2811688	-0.3571639	-4.2634913

C	3.9451316	0.6320670	-3.5148684
C	1.6928661	0.9285470	-0.4551222
C	2.3191426	0.5048992	0.7672914
C	3.4954253	-0.4220752	0.6106261
C	3.3485364	-1.7336595	0.1085057
C	4.4610434	-2.5629159	-0.0889554
C	5.7504790	-2.1020734	0.2249429
C	5.9135100	-0.8019141	0.7293926
C	4.7985285	0.0302489	0.9156008
Br	0.9933053	2.8283601	-0.6628729
C	0.7160305	-0.6722179	3.1056955
C	-0.4930444	-0.0459858	3.7564465
C	0.6560732	-1.9267612	2.5503953
C	2.0378424	0.0849048	3.2367997
C	2.2422366	1.1800016	2.1624562
O	1.2059752	2.1292837	2.3325356
H	3.2310655	1.6673761	2.3639189
H	2.0813640	0.5755525	4.2321506
H	2.8876795	-0.6217900	3.1742809
H	1.5685807	-2.4417426	2.2116929
H	-0.2861820	-2.4972274	2.5479601
H	-0.5703657	1.0237098	3.4880357
H	-0.3784431	-0.0908757	4.8624241
H	-1.4293981	-0.5691818	3.4814155
H	1.1896415	2.7095254	1.5369276
H	2.3349496	-2.0875033	-0.1367847
H	4.3185269	-3.5777994	-0.4903377
H	6.6252484	-2.7527159	0.0746392
H	6.9195425	-0.4255073	0.9707634
H	4.9471831	1.0560553	1.2848217
H	0.6377879	-0.9234336	-2.1449081
H	1.5572975	-1.6852795	-4.3558465
H	3.6981311	-0.6934013	-5.2251720
H	4.8852065	1.0671635	-3.8870348
H	3.9324259	1.8366612	-1.7044438
Pd	0.3526980	-0.3481847	0.5470225
P	-1.8292811	-0.4285301	-0.1045413
C	-2.7157674	1.1372510	0.2757856
C	-2.0999613	2.0647153	1.1388027
H	-1.0944816	1.8480087	1.5335526
C	-2.7504522	3.2680490	1.4553119
H	-2.2606324	3.9906175	2.1254303
C	-4.0110660	3.5531651	0.9064068
H	-4.5179252	4.4993734	1.1505699
C	-4.6216546	2.6357298	0.0319343
H	-5.6042286	2.8636152	-0.4089248

C	-3.9758137	1.4320961	-0.2868352
H	-4.4448246	0.7192721	-0.9826123
C	-2.8230097	-1.7348886	0.7294695
C	-3.9671699	-1.4686788	1.5071545
H	-4.3526752	-0.4411672	1.5783289
C	-4.6100258	-2.5104907	2.1977691
H	-5.4991087	-2.2904552	2.8083653
C	-4.1247081	-3.8248857	2.1109428
H	-4.6315929	-4.6382482	2.6518707
C	-2.9814007	-4.0972911	1.3378510
H	-2.5906007	-5.1241263	1.2716514
C	-2.3265897	-3.0571804	0.6637670
H	-1.4102338	-3.2616374	0.0864583
C	-2.2031691	-0.6404766	-1.8953208
C	-2.9509758	-1.7093746	-2.4252719
H	-3.3955888	-2.4564881	-1.7512150
C	-3.1320141	-1.8195977	-3.8151096
H	-3.7168072	-2.6585717	-4.2226086
C	-2.5758651	-0.8633700	-4.6797328
H	-2.7180780	-0.9536775	-5.7673756
C	-1.8356395	0.2103595	-4.1518845
H	-1.3925944	0.9615181	-4.8229042
C	-1.6448354	0.3207052	-2.7686878
H	-1.0506641	1.1518637	-2.3561129

Optimized Geometries(MXna)

R1
75
SCF Energy = -4548.292050107

C	-2.6846013	-1.4370333	-0.8410769
C	-2.2592360	-2.1821057	0.2839907
C	-3.0304906	-3.2970843	0.6797397
C	-4.1752743	-3.6688130	-0.0410003
C	-4.5779804	-2.9295927	-1.1655217
C	-3.8278997	-1.8083984	-1.5592231
C	-0.9907085	-1.8189482	0.9820318
C	0.3053591	-1.7924689	0.3846939
C	0.4674222	-2.0525754	-1.0911550
C	-0.1992548	-3.1069907	-1.7539578
C	-0.0053125	-3.3366857	-3.1230636
C	0.8622963	-2.5207191	-3.8669300
C	1.5260813	-1.4622304	-3.2261632
C	1.3245673	-1.2273417	-1.8598648

Br	-1.1168954	-2.0418960	2.9401766
C	1.9284371	-4.4429039	0.5878985
C	0.7438970	-5.3595522	0.4233496
C	3.0181828	-4.5146513	-0.2089499
C	1.8301775	-3.4369114	1.7134123
C	1.5815318	-1.9715310	1.2495227
O	2.7399685	-1.4575262	0.6151987
H	1.4511938	-1.3675509	2.1679737
H	1.0237284	-3.7205668	2.4178641
H	2.7757449	-3.3992427	2.2923851
H	3.9099660	-3.8960511	-0.0195356
H	3.0630901	-5.2131243	-1.0592458
H	-0.2124388	-4.8015801	0.4878721
H	0.7233313	-6.0950400	1.2579562
H	0.7678151	-5.9183927	-0.5316635
H	2.8558617	-1.9693982	-0.2144640
H	-0.8846253	-3.7543823	-1.1954997
H	-0.5417305	-4.1643306	-3.6118152
H	1.0095210	-2.7006500	-4.9427326
H	2.1858845	-0.7905042	-3.7944440
H	1.8034640	-0.3649154	-1.3815979
H	-2.7233223	-3.8740523	1.5642136
H	-4.7587358	-4.5445458	0.2819533
H	-5.4788493	-3.2203425	-1.7268729
H	-4.1373443	-1.2135690	-2.4319333
H	-2.0838081	-0.5633084	-1.1414696
Pd	-0.4218709	0.2184212	0.6609478
P	0.3730803	2.1909376	-0.1274927
C	-0.7119049	3.6657632	0.0701518
C	-0.8607099	4.6463797	-0.9317210
H	-0.3279064	4.5347129	-1.8879626
C	-1.6904300	5.7575589	-0.7102830
H	-1.8054486	6.5184339	-1.4973838
C	-2.3720844	5.8984582	0.5101533
H	-3.0235855	6.7691351	0.6798343
C	-2.2281185	4.9218498	1.5110794
H	-2.7665613	5.0247475	2.4653590
C	-1.4067117	3.8065348	1.2902067
H	-1.3005905	3.0288969	2.0642971
C	2.0106113	2.7758553	0.4729532
C	2.9828508	1.7982280	0.7766225
H	2.7458326	0.7246191	0.6834778
C	4.2615956	2.1947910	1.1977587
H	5.0148423	1.4266085	1.4299292
C	4.5732003	3.5584938	1.3348860
H	5.5741212	3.8651510	1.6753707

C	3.6015384	4.5309058	1.0441142
H	3.8387817	5.6000205	1.1559443
C	2.3231868	4.1435295	0.6108624
H	1.5642498	4.9067042	0.3826885
C	0.6048056	2.0922531	-1.9546279
C	-0.4734027	1.6012123	-2.7221468
H	-1.4127905	1.3258753	-2.2172974
C	-0.3466180	1.4496166	-4.1080912
H	-1.1916683	1.0602371	-4.6952383
C	0.8667470	1.7708934	-4.7428009
H	0.9724378	1.6375579	-5.8300683
C	1.9459497	2.2497801	-3.9835777
H	2.8991560	2.4987213	-4.4746716
C	1.8172577	2.4153169	-2.5929959
H	2.6645989	2.7904257	-2.0004390

R2

75

SCF Energy = -4548.290435118

C	-2.1914992	-1.4356451	-2.0633908
C	-2.4281646	-1.9926086	-0.7807170
C	-3.5230198	-2.8708171	-0.6282051
C	-4.3423479	-3.1952315	-1.7202610
C	-4.0906181	-2.6450709	-2.9870934
C	-3.0102259	-1.7609316	-3.1511518
C	-1.5084695	-1.6628986	0.3463300
C	-0.0881075	-1.7419169	0.2934212
C	0.5708083	-2.2370816	-0.9637081
C	0.2029853	-3.4762224	-1.5313374
C	0.8771114	-3.9744450	-2.6536622
C	1.9336523	-3.2476418	-3.2309838
C	2.2983319	-2.0065079	-2.6862330
C	1.6177717	-1.5030004	-1.5655888
Br	-2.3775494	-1.6906735	2.1129836
C	1.3235095	-4.4372430	1.3069754
C	2.7227723	-4.3445507	0.7479880
C	0.5493906	-5.5228777	1.0930553
C	0.8190433	-3.2957633	2.1605454
C	0.7760037	-1.8599366	1.5672547
O	2.0751051	-1.3098968	1.3938476
H	0.2956370	-1.2332884	2.3435964
H	-0.2006333	-3.5339445	2.5246110
H	1.4703077	-3.2068368	3.0594160
H	-0.4743245	-5.5836321	1.4956674
H	0.9109072	-6.3794839	0.5017271
H	3.4437065	-3.9973277	1.5166629

H	2.7708363	-3.6172959	-0.0915606
H	3.0661576	-5.3184620	0.3486901
H	2.4242549	-1.6318188	0.5376831
H	-0.6123324	-4.0533516	-1.0773931
H	0.5760538	-4.9431414	-3.0806276
H	2.4616406	-3.6444682	-4.1114801
H	3.1063193	-1.4100647	-3.1354557
H	1.8658754	-0.5080169	-1.1755715
H	-3.7282691	-3.3024929	0.3617018
H	-5.1873204	-3.8857724	-1.5760248
H	-4.7373163	-2.8973865	-3.8410939
H	-2.8035998	-1.3144698	-4.1356442
H	-1.3469892	-0.7400067	-2.1888124
Pd	-0.7264129	0.3214128	0.1605031
P	0.4365941	2.2468227	-0.1111120
C	0.7372433	3.2768107	1.3830222
C	1.8583639	4.1217795	1.5217902
H	2.6224112	4.1534182	0.7302192
C	2.0108577	4.9039923	2.6774543
H	2.8898389	5.5581735	2.7824475
C	1.0480799	4.8484327	3.6997469
H	1.1724527	5.4599453	4.6063632
C	-0.0656616	4.0013711	3.5698486
H	-0.8140566	3.9445607	4.3746454
C	-0.2173940	3.2132672	2.4188923
H	-1.0716821	2.5238142	2.3170105
C	2.1282467	1.9454887	-0.7675279
C	2.4351567	2.1317874	-2.1302597
H	1.6902810	2.5826835	-2.8025113
C	3.6843272	1.7297556	-2.6321119
H	3.9139804	1.8744346	-3.6988053
C	4.6352318	1.1468715	-1.7786353
H	5.6122563	0.8303426	-2.1740604
C	4.3330945	0.9662009	-0.4165257
H	5.0703129	0.5033559	0.2569285
C	3.0851718	1.3559274	0.0890001
H	2.8344599	1.1613173	1.1412791
C	-0.2870364	3.4229726	-1.3340478
C	-1.2372271	2.9125819	-2.2429831
H	-1.5336165	1.8530606	-2.1632720
C	-1.7981424	3.7457486	-3.2240237
H	-2.5393784	3.3392092	-3.9286145
C	-1.4202556	5.0965866	-3.2961512
H	-1.8637772	5.7530763	-4.0602298
C	-0.4817570	5.6127912	-2.3850825
H	-0.1910509	6.6732498	-2.4348063

C	0.0844306	4.7808326	-1.4074258
H	0.8123027	5.1912072	-0.6918685

R3

75

SCF Energy = -4548.290223003

C	-1.2690978	2.5226400	-0.9456155
C	-2.1995438	2.0646399	0.0192992
C	-3.3165250	2.8800267	0.3079599
C	-3.5107711	4.0958499	-0.3652192
C	-2.5876027	4.5304802	-1.3304388
C	-1.4612450	3.7385297	-1.6118868
C	-2.0049900	0.7334734	0.6701485
C	-1.8361730	-0.5008910	-0.0233524
C	-1.8231738	-0.5282571	-1.5277234
C	-2.8348192	0.0944617	-2.2914100
C	-2.8274898	0.0200639	-3.6920598
C	-1.8192378	-0.6917263	-4.3634916
C	-0.8127751	-1.3269621	-3.6179528
C	-0.8123270	-1.2407591	-2.2169674
Br	-2.6104913	0.6928211	2.5423481
C	-4.7561791	-1.6851601	0.9240139
C	-5.3171579	-0.4587034	0.2523609
C	-5.2718884	-2.1609655	2.0767989
C	-3.5869127	-2.3842396	0.2598924
C	-2.1656561	-1.8631129	0.6192583
O	-1.2079272	-2.8617183	0.2798998
H	-2.1016203	-1.7531280	1.7177184
H	-3.5747842	-3.4491729	0.5666295
H	-3.6988006	-2.3630442	-0.8470757
H	-4.8651370	-3.0650257	2.5578057
H	-6.1091823	-1.6555613	2.5836169
H	-5.6318875	-0.6870529	-0.7885647
H	-4.5572913	0.3457034	0.1810867
H	-6.1879764	-0.0523012	0.8012978
H	-1.2016323	-2.9393582	-0.6962090
H	-3.6281360	0.6550091	-1.7810519
H	-3.6201060	0.5260133	-4.2641025
H	-1.8160629	-0.7460500	-5.4626544
H	-0.0045480	-1.8772942	-4.1230736
H	0.0179479	-1.6789148	-1.6466540
H	-4.0346403	2.5550192	1.0742315
H	-4.3915064	4.7113686	-0.1264838
H	-2.7383666	5.4887354	-1.8504005
H	-0.7140683	4.0694220	-2.3490800
H	-0.3798343	1.9104094	-1.1560994

Pd	0.0590760	0.2269188	0.7378367
P	2.1976568	-0.1875147	0.1071065
C	3.6053217	-0.1516094	1.2917995
C	3.4281289	0.5520979	2.5002074
H	2.4509556	1.0162859	2.7130765
C	4.4822351	0.6498539	3.4221164
H	4.3378041	1.2015240	4.3633346
C	5.7139678	0.0322664	3.1470653
H	6.5381855	0.1002686	3.8733179
C	5.8909362	-0.6809834	1.9483820
H	6.8532783	-1.1711404	1.7355976
C	4.8417770	-0.7725112	1.0209270
H	4.9790407	-1.3323052	0.0833246
C	2.4369359	-1.7739988	-0.7948466
C	1.8663366	-2.9317882	-0.2235930
H	1.2879803	-2.8492995	0.7082049
C	1.9794879	-4.1665922	-0.8785772
H	1.5218080	-5.0617746	-0.4312066
C	2.6523286	-4.2545604	-2.1102421
H	2.7284277	-5.2220711	-2.6294999
C	3.2206521	-3.1036715	-2.6812805
H	3.7478302	-3.1680412	-3.6455007
C	3.1180829	-1.8652623	-2.0256713
H	3.5569039	-0.9637889	-2.4783033
C	2.6602498	1.0919835	-1.1392034
C	3.7230087	1.9951751	-0.9450874
H	4.3630939	1.9050635	-0.0551263
C	3.9623408	3.0149374	-1.8828898
H	4.7915007	3.7200232	-1.7186839
C	3.1512120	3.1359074	-3.0218084
H	3.3413246	3.9361187	-3.7530699
C	2.0936635	2.2299467	-3.2244126
H	1.4521641	2.3133919	-4.1148989
C	1.8437385	1.2189927	-2.2873523
H	1.0083571	0.5202445	-2.4462719

R4

75

SCF Energy = -4548.292500606

C	-1.4434597	0.3573793	-2.6568184
C	-2.3706907	0.8504278	-1.7117899
C	-3.6493207	1.2486041	-2.1611973
C	-3.9969311	1.1293440	-3.5141943
C	-3.0723863	0.6206976	-4.4437186
C	-1.7923994	0.2399037	-4.0092285
C	-2.0262716	0.8803327	-0.2590292

C	-1.7972808	-0.2687066	0.5494574
C	-1.7894868	-1.6377770	-0.0766395
C	-2.8024532	-2.0656952	-0.9633307
C	-2.7884027	-3.3615902	-1.5006670
C	-1.7724958	-4.2680201	-1.1540119
C	-0.7644066	-3.8622439	-0.2642096
C	-0.7708088	-2.5617176	0.2627337
Br	-2.5440974	2.5806574	0.5918626
C	-4.6362138	0.0841390	1.9812392
C	-4.9163438	1.2336456	2.9166604
C	-5.3709904	-0.1353551	0.8706406
C	-3.4926452	-0.8246042	2.3729745
C	-2.0704404	-0.2729609	2.0661803
O	-1.1021309	-1.0040096	2.8079297
H	-1.9923820	0.7683445	2.4309902
H	-3.5076875	-0.9973594	3.4703801
H	-3.5964575	-1.8145613	1.8812296
H	-5.1798327	-1.0016992	0.2198321
H	-6.1942647	0.5385197	0.5851070
H	-4.0016370	1.8326177	3.1062524
H	-5.2595299	0.8532406	3.9037263
H	-5.6924120	1.9137253	2.5164234
H	-1.1012622	-1.9198913	2.4618006
H	-3.6009337	-1.3683667	-1.2461293
H	-3.5830533	-3.6642947	-2.1995541
H	-1.7642021	-5.2827173	-1.5800170
H	0.0521207	-4.5476448	0.0088811
H	0.0631950	-2.2317353	0.8960853
H	-4.3720568	1.6415855	-1.4315327
H	-5.0007197	1.4359493	-3.8461423
H	-3.3478917	0.5315075	-5.5056349
H	-1.0516818	-0.1477146	-4.7250321
H	-0.4418725	0.0610735	-2.3070804
Pd	0.0633933	0.7396903	0.1117240
P	2.2071295	-0.0029281	0.1227525
C	3.6507183	1.0604364	0.5357157
C	4.8844377	0.5310681	0.9666312
H	4.9973877	-0.5561681	1.0953511
C	5.9612774	1.3900823	1.2352326
H	6.9214401	0.9734660	1.5760688
C	5.8146735	2.7787213	1.0718067
H	6.6604075	3.4499804	1.2853016
C	4.5857992	3.3103928	0.6453273
H	4.4655704	4.3976816	0.5249210
C	3.5043519	2.4543003	0.3850961
H	2.5297329	2.8613391	0.0689458

C	2.4627367	-1.4930304	1.1729995
C	1.9905393	-1.4331671	2.5020562
H	1.4908792	-0.5214808	2.8607788
C	2.0991492	-2.5538843	3.3373647
H	1.7169506	-2.5014921	4.3679051
C	2.6678341	-3.7450092	2.8516088
H	2.7380735	-4.6288079	3.5038509
C	3.1391299	-3.8072779	1.5297987
H	3.5852050	-4.7373920	1.1455081
C	3.0420682	-2.6840349	0.6910672
H	3.4034869	-2.7372711	-0.3463584
C	2.5929466	-0.6026299	-1.5790487
C	1.6861556	-1.5126268	-2.1715704
H	0.8211951	-1.8761485	-1.5959448
C	1.8862487	-1.9541942	-3.4860316
H	1.1748172	-2.6657491	-3.9319373
C	2.9827491	-1.4820064	-4.2309166
H	3.1338892	-1.8207622	-5.2671225
C	3.8823367	-0.5758161	-3.6481026
H	4.7414741	-0.2023686	-4.2261066
C	3.6934029	-0.1387966	-2.3251313
H	4.4023657	0.5704072	-1.8732305

S1

75

SCF Energy = -4548.293023754

C	-1.5648398	2.1185703	-1.8476853
C	-2.4292154	1.9321089	-0.7432711
C	-3.7233299	2.4964733	-0.8014567
C	-4.1500916	3.1933249	-1.9414350
C	-3.2903454	3.3490516	-3.0421522
C	-1.9929671	2.8127828	-2.9867919
C	-1.9850971	1.1091022	0.4225485
C	-1.7354926	-0.3003362	0.4308820
C	-1.8208098	-1.1161774	-0.8328552
C	-2.7186323	-0.8363084	-1.8879020
C	-2.7500748	-1.6348815	-3.0409572
C	-1.8903573	-2.7363238	-3.1740475
C	-1.0005341	-3.0368469	-2.1281718
C	-0.9706957	-2.2412964	-0.9787264
Br	-2.5135291	1.9892518	2.1365042
C	-4.1371744	-2.0345020	1.0914453
C	-5.1038446	-1.0590962	0.4728426
C	-4.0488847	-3.3201520	0.6945652
C	-3.2376538	-1.4794319	2.1783220
C	-1.7857507	-1.1672498	1.7165575

O	-1.0101313	-0.7004247	2.8072520
H	-1.3226669	-2.1327734	1.4379002
H	-3.6741236	-0.5509553	2.5990408
H	-3.1364131	-2.1995200	3.0155915
H	-3.3392592	-4.0191041	1.1659562
H	-4.6659593	-3.7124991	-0.1285943
H	-4.5815788	-0.1380383	0.1396591
H	-5.8566946	-0.7296526	1.2222251
H	-5.6375099	-1.4897417	-0.3958993
H	-1.3442493	0.1941511	3.0377434
H	-3.4155566	0.0049715	-1.8098723
H	-3.4637895	-1.3904460	-3.8425341
H	-1.9152695	-3.3571744	-4.0823626
H	-0.3101317	-3.8898281	-2.2082494
H	-0.2450886	-2.4780411	-0.1907869
H	-4.3991107	2.3833583	0.0589146
H	-5.1649413	3.6185968	-1.9690289
H	-3.6273279	3.8974428	-3.9348701
H	-1.3027000	2.9378642	-3.8346827
H	-0.5498977	1.6884443	-1.7937135
C	3.8378079	1.9428628	0.8187829
C	3.7149151	0.5434219	0.6881756
C	4.7773771	-0.2882293	1.0954027
C	5.9518699	0.2768886	1.6187464
C	6.0748066	1.6715297	1.7338203
C	5.0159937	2.5046812	1.3316165
P	2.1534257	-0.1106893	-0.0323442
C	2.5024723	-0.1274661	-1.8434259
C	3.7929111	0.0508752	-2.3801351
C	3.9870404	0.0114282	-3.7715123
C	2.8995771	-0.2128547	-4.6319142
C	1.6104862	-0.3919813	-4.0991701
C	1.4096486	-0.3405777	-2.7129948
Pd	0.1159959	0.7966902	0.4169406
C	2.1817638	-1.8964163	0.4150807
C	2.6696850	-2.8901213	-0.4562437
C	2.5805825	-4.2450265	-0.0946641
C	2.0123979	-4.6117337	1.1365090
C	1.5322051	-3.6194505	2.0101919
C	1.6083539	-2.2656233	1.6517628
H	3.0995935	-2.6041779	-1.4275482
H	2.9521173	-5.0188754	-0.7837385
H	1.9349367	-5.6744086	1.4124638
H	1.0734452	-3.9007615	2.9702144
H	1.1659800	-1.4947563	2.3035242
H	4.6470422	0.2241649	-1.7085664

H	4.9968445	0.1570549	-4.1849168
H	3.0564252	-0.2440126	-5.7209663
H	0.7509373	-0.5681312	-4.7631328
H	0.4017333	-0.4769607	-2.2938664
H	4.6809462	-1.3806382	1.0049918
H	6.7765254	-0.3778485	1.9394825
H	6.9957733	2.1114493	2.1456127
H	5.1051036	3.5973649	1.4283816
H	2.9972235	2.5899704	0.5189321

S2

75

SCF Energy = -4548.295735503

C	-2.0212436	-1.6529027	-1.9382687
C	-1.9174326	-2.4516900	-0.7752098
C	-2.5306096	-3.7239689	-0.7767388
C	-3.2004077	-4.1938250	-1.9156625
C	-3.2778330	-3.3997731	-3.0727104
C	-2.6881794	-2.1247555	-3.0764495
C	-1.1229527	-1.9664785	0.3922854
C	0.2849956	-1.7296826	0.4125855
C	1.0991316	-1.8962125	-0.8434766
C	0.8845974	-2.9436126	-1.7653522
C	1.6863631	-3.0681934	-2.9092459
C	2.7274602	-2.1580569	-3.1565534
C	2.9666847	-1.1229687	-2.2364536
C	2.1651430	-0.9987255	-1.0944004
Br	-2.0505930	-2.3673727	2.1106941
C	1.8048645	-4.2385876	1.1776097
C	3.2084289	-4.0970571	0.6474553
C	0.9684989	-5.2124874	0.7600455
C	1.3536224	-3.2281571	2.2059904
C	1.1538812	-1.7714787	1.6951162
O	0.7279131	-0.9429648	2.7644017
H	2.1393218	-1.3607866	1.4000641
H	0.3954701	-3.5593841	2.6517683
H	2.0931695	-3.1582528	3.0332026
H	-0.0539927	-5.2959313	1.1611027
H	1.2760676	-5.9484666	0.0003373
H	3.9490504	-4.1412303	1.4752787
H	3.3505387	-3.1170625	0.1443796
H	3.4537079	-4.8887237	-0.0858664
H	-0.1849051	-1.2215072	2.9967738
H	0.0979494	-3.6823111	-1.5735650
H	1.4970966	-3.8943033	-3.6116035
H	3.3525251	-2.2588664	-4.0568020

H	3.7757349	-0.3971222	-2.4080194
H	2.3484465	-0.1712769	-0.3961538
H	-2.4712721	-4.3500445	0.1253612
H	-3.6650415	-5.1915419	-1.8988676
H	-3.8055976	-3.7703960	-3.9645518
H	-2.7510680	-1.4856321	-3.9701016
H	-1.5539799	-0.6534244	-1.9293011
Pd	-0.7960328	0.1309051	0.3301157
P	0.0952349	2.1813277	-0.0814313
C	1.8901538	2.2248593	0.3287302
C	2.8555370	2.7657981	-0.5436128
H	2.5411841	3.2210094	-1.4945036
C	4.2185145	2.7018039	-0.2078467
H	4.9700334	3.1163777	-0.8971199
C	4.6213272	2.1058631	0.9986424
H	5.6902894	2.0495801	1.2548920
C	3.6574494	1.5714078	1.8724267
H	3.9675630	1.0915418	2.8131210
C	2.2957781	1.6221126	1.5399262
H	1.5478857	1.1420054	2.1922943
C	-0.5663260	3.7075420	0.7048049
C	0.2548562	4.7835651	1.0975026
H	1.3442194	4.7189176	0.9561653
C	-0.3165132	5.9306888	1.6719400
H	0.3300938	6.7660057	1.9813992
C	-1.7072861	6.0125118	1.8530775
H	-2.1520179	6.9120328	2.3051674
C	-2.5296783	4.9399904	1.4657590
H	-3.6186745	4.9967065	1.6143563
C	-1.9609012	3.7887909	0.9015282
H	-2.5979568	2.9366276	0.6131074
C	0.0709093	2.5887626	-1.8798733
C	0.3340109	1.5354158	-2.7841755
H	0.5379609	0.5255386	-2.3960735
C	0.3480000	1.7776113	-4.1645207
H	0.5623408	0.9501617	-4.8576583
C	0.0810209	3.0679154	-4.6568963
H	0.0819644	3.2562519	-5.7413558
C	-0.1921047	4.1150196	-3.7617799
H	-0.4058165	5.1252997	-4.1431048
C	-0.1937523	3.8802528	-2.3758932
H	-0.4048429	4.7032533	-1.6770036

S3

75

SCF Energy = -4548.292490475

C	-1.2292298	-1.7603029	-2.3919935
C	-1.6422387	-2.3949630	-1.1934217
C	-2.5208745	-3.4960380	-1.2919280
C	-2.9559627	-3.9598311	-2.5431260
C	-2.5287872	-3.3300732	-3.7226270
C	-1.6644254	-2.2245706	-3.6384220
C	-1.1095855	-1.9160089	0.1180855
C	0.2751750	-1.7494901	0.4210206
C	1.3037851	-2.0988165	-0.6219757
C	1.2692899	-3.3264059	-1.3181701
C	2.2653608	-3.6481771	-2.2517271
C	3.3195515	-2.7539189	-2.5008549
C	3.3744138	-1.5371414	-1.8001709
C	2.3771466	-1.2161784	-0.8699065
Br	-2.4241989	-2.1538073	1.5856205
C	0.3398923	-4.0548467	2.7249595
C	-0.1802222	-5.0012842	1.6738672
C	-0.1514143	-4.0367404	3.9831711
C	1.4314654	-3.0916621	2.3127804
C	0.9294229	-1.6972767	1.8218503
O	0.2129399	-1.0193968	2.8282190
H	1.8470974	-1.0914628	1.6687141
H	2.0876199	-2.8798515	3.1806010
H	2.0662516	-3.5325238	1.5166976
H	0.2493066	-3.3472513	4.7426328
H	-0.9685400	-4.7087679	4.2903668
H	0.6420972	-5.6302033	1.2698356
H	-0.6030586	-4.4480969	0.8099438
H	-0.9704618	-5.6666457	2.0708554
H	-0.6575602	-1.4660546	2.9253269
H	0.4493355	-4.0326407	-1.1315142
H	2.2149613	-4.6075797	-2.7888184
H	4.0966009	-3.0049839	-3.2388290
H	4.1875012	-0.8205086	-1.9862064
H	2.4071305	-0.2488738	-0.3489851
H	-2.8658005	-3.9922768	-0.3736224
H	-3.6378466	-4.8224543	-2.5928229
H	-2.8749081	-3.6920164	-4.7025973
H	-1.3283746	-1.7131431	-4.5531034
H	-0.5540906	-0.8931250	-2.3198273
Pd	-0.6759959	0.1607372	0.0620652
P	0.2560333	2.2165567	-0.1468140
C	-0.7882325	3.5825584	-0.8119865
C	-0.3162608	4.5355298	-1.7373513
H	0.7142085	4.4659517	-2.1171687
C	-1.1627577	5.5645868	-2.1814902

H	-0.7888653	6.3039446	-2.9062509
C	-2.4812866	5.6504408	-1.7048704
H	-3.1430616	6.4564703	-2.0564815
C	-2.9573086	4.6999323	-0.7848206
H	-3.9922487	4.7586065	-0.4151576
C	-2.1171159	3.6668253	-0.3447998
H	-2.4888684	2.9107249	0.3660404
C	0.9889803	2.9551424	1.3702966
C	1.1358622	2.1321610	2.5058447
H	0.7670368	1.0920424	2.4868934
C	1.7249590	2.6524309	3.6707923
H	1.8345075	2.0061627	4.5548668
C	2.1584675	3.9874272	3.7105795
H	2.6154089	4.3926781	4.6264899
C	1.9971541	4.8128266	2.5829028
H	2.3246790	5.8632586	2.6156573
C	1.4119003	4.3007131	1.4156220
H	1.2763002	4.9500328	0.5370797
C	1.6588935	2.1540574	-1.3398439
C	1.3823555	1.6737719	-2.6395232
H	0.3476935	1.4086822	-2.9092082
C	2.4136678	1.5235736	-3.5742511
H	2.1865007	1.1483728	-4.5833492
C	3.7393166	1.8308534	-3.2166976
H	4.5519158	1.7006082	-3.9472712
C	4.0227193	2.2913019	-1.9216767
H	5.0587559	2.5261527	-1.6333640
C	2.9869591	2.4577487	-0.9846742
H	3.2140249	2.8192537	0.0288597

S4

75

SCF Energy = -4548.292218918

C	-1.4173632	-1.7593368	-2.3587005
C	-1.6559522	-2.4452917	-1.1454015
C	-2.3535109	-3.6722633	-1.1901978
C	-2.7804975	-4.2062391	-2.4145927
C	-2.5245581	-3.5230886	-3.6157654
C	-1.8428932	-2.2952319	-3.5812295
C	-1.1203385	-1.9009441	0.1376084
C	0.2614637	-1.7236258	0.4444959
C	1.2989427	-2.0323732	-0.6049865
C	1.2520147	-3.1985751	-1.3992938
C	2.2599951	-3.4679075	-2.3375233
C	3.3396438	-2.5842407	-2.4948661
C	3.4080886	-1.4297613	-1.6963952

C	2.3995119	-1.1601386	-0.7635388
Br	-2.4523928	-2.0902542	1.6025430
C	0.2086449	-4.1350467	2.5221225
C	-0.4579938	-4.0766765	3.8738909
C	-0.1508591	-5.0291035	1.5765771
C	1.3277105	-3.1456553	2.2850868
C	0.8976751	-1.7093686	1.8513807
O	0.1960802	-1.0105917	2.8637153
H	1.8482782	-1.1492492	1.7271888
H	1.9213779	-3.0164558	3.2151391
H	2.0157048	-3.5290462	1.5050676
H	0.3737713	-5.0821974	0.6106395
H	-0.9778861	-5.7378205	1.7418950
H	-0.7450590	-3.0374690	4.1301653
H	0.2535583	-4.4009539	4.6651457
H	-1.3551737	-4.7228548	3.9270185
H	-0.7616676	-1.2146671	2.7672795
H	0.4152189	-3.8995200	-1.2863973
H	2.1983821	-4.3810176	-2.9490189
H	4.1259928	-2.7946423	-3.2356666
H	4.2410136	-0.7207455	-1.8088825
H	2.4437233	-0.2380172	-0.1669580
H	-2.5461444	-4.2122907	-0.2519014
H	-3.3161835	-5.1677245	-2.4300060
H	-2.8627437	-3.9434251	-4.5750374
H	-1.6436207	-1.7456673	-4.5136571
H	-0.8756224	-0.7998149	-2.3149556
Pd	-0.6748880	0.1757365	0.0478546
P	0.2850180	2.2226577	-0.1653717
C	1.0315383	2.9519920	1.3493235
C	1.1972933	2.1207188	2.4763047
H	0.8301190	1.0796765	2.4568386
C	1.7997122	2.6342524	3.6372890
H	1.9229989	1.9815657	4.5148158
C	2.2279366	3.9708559	3.6821167
H	2.6951941	4.3708009	4.5951369
C	2.0473184	4.8045831	2.5636498
H	2.3701110	5.8563361	2.6005848
C	1.4486450	4.2992325	1.4001148
H	1.2977153	4.9549329	0.5288299
C	1.6842863	2.1393456	-1.3622236
C	1.4063338	1.6162527	-2.6445229
H	0.3764284	1.3152707	-2.8938921
C	2.4304183	1.4673023	-3.5873506
H	2.2020231	1.0567638	-4.5822267
C	3.7509019	1.8196958	-3.2543847

H	4.5585333	1.6904541	-3.9906238
C	4.0368060	2.3220453	-1.9754935
H	5.0695507	2.5912841	-1.7059855
C	3.0078680	2.4861138	-1.0307417
H	3.2370056	2.8806760	-0.0300954
C	-0.7388854	3.6042922	-0.8300353
C	-0.2603484	4.5350845	-1.7743110
H	0.7629317	4.4388111	-2.1674185
C	-1.0912131	5.5766250	-2.2191052
H	-0.7123488	6.2985993	-2.9586530
C	-2.4002493	5.6970405	-1.7243233
H	-3.0497205	6.5128155	-2.0763928
C	-2.8827944	4.7686048	-0.7852273
H	-3.9105327	4.8544969	-0.4010618
C	-2.0586336	3.7230239	-0.3445383
H	-2.4359739	2.9841541	0.3812931

Optimized Geometries(BXn)(TS_ab)

R1
75
SCF Energy = -4548.282020320

C	-0.0033402	3.1504773	-2.4617977
C	-0.6039805	3.0507396	-1.1798409
C	-1.9951350	3.3013134	-1.0900147
C	-2.7666073	3.5684467	-2.2249633
C	-2.1663982	3.6006180	-3.4952775
C	-0.7789448	3.4018530	-3.6011342
C	0.2029966	2.7173994	0.0104529
C	1.4840137	2.2086311	0.0672392
C	1.8870636	1.2973325	-1.0450021
C	1.0494015	0.2075806	-1.3686888
C	1.3714436	-0.6612951	-2.4205118
C	2.5501861	-0.4636081	-3.1573137
C	3.4111242	0.5979400	-2.8203117
C	3.0900389	1.4668666	-1.7694206
Br	-0.4885563	4.4980925	1.5251241
C	1.1069495	1.9539362	3.2408426
C	0.6250275	2.5323557	4.5561282
C	0.8017463	0.6325887	2.9122706
C	2.1616378	2.7994342	2.5510804
C	2.5859618	2.4007908	1.1339902
O	3.4830527	1.2924201	1.1644381
H	3.2150340	3.2362470	0.7466031

H	1.8120963	3.8513628	2.5472442
H	3.0926073	2.7875059	3.1632782
H	1.3070697	0.0763614	2.1061853
H	0.2293265	0.0134566	3.6206234
H	0.2473033	3.5657415	4.4191992
H	1.4665013	2.5843898	5.2829040
H	-0.1805349	1.9203116	5.0060067
H	2.9968194	0.5375895	1.5458174
H	0.1385890	0.0493915	-0.7744234
H	0.6947529	-1.4964167	-2.6574952
H	2.8083943	-1.1414167	-3.9851083
H	4.3438184	0.7496480	-3.3850227
H	3.7668322	2.2958088	-1.5171280
H	-2.4686770	3.2934393	-0.1042425
H	-3.8463485	3.7447713	-2.1085981
H	-2.7700975	3.7990097	-4.3937918
H	-0.2863818	3.4517778	-4.5841316
H	1.0784662	3.0084727	-2.5686730
Pd	-0.6516427	1.8983741	1.7276946
P	-2.5858638	0.7202718	1.2007791
C	-4.1208426	1.7226909	1.0037005
C	-4.1874869	2.9521114	1.6944289
H	-3.3249411	3.2763772	2.3000502
C	-5.3213693	3.7686111	1.5743570
H	-5.3625720	4.7275550	2.1125564
C	-6.3900595	3.3719765	0.7512838
H	-7.2741060	4.0190462	0.6456628
C	-6.3230398	2.1531967	0.0552953
H	-7.1557773	1.8424647	-0.5941142
C	-5.1943958	1.3269530	0.1822387
H	-5.1420971	0.3743349	-0.3652436
C	-2.7054446	-0.4810207	-0.1992584
C	-3.1978267	-1.7935780	-0.0367383
H	-3.5318512	-2.1362926	0.9528735
C	-3.2666070	-2.6660236	-1.1351685
H	-3.6502070	-3.6880012	-0.9931662
C	-2.8546017	-2.2379807	-2.4080515
H	-2.9090771	-2.9246428	-3.2665259
C	-2.3763089	-0.9279212	-2.5788775
H	-2.0523557	-0.5757398	-3.5695816
C	-2.2981668	-0.0561420	-1.4831500
H	-1.9245133	0.9651199	-1.6286040
C	-2.9818227	-0.3316328	2.6645151
C	-2.0659927	-1.3505132	3.0149582
H	-1.1796540	-1.5209200	2.3847361
C	-2.2868936	-2.1467859	4.1464008

H	-1.5715928	-2.9435020	4.4016502
C	-3.4147485	-1.9228204	4.9574299
H	-3.5826189	-2.5402694	5.8527205
C	-4.3241520	-0.9089686	4.6182319
H	-5.2106954	-0.7305638	5.2457938
C	-4.1154774	-0.1201672	3.4737572
H	-4.8380042	0.6649022	3.2081187

R2

75

SCF Energy = -4548.283554630

C	-0.1164826	2.6324972	-3.0528838
C	-0.9264759	2.9692057	-1.9406951
C	-2.2938703	3.2526055	-2.1831190
C	-2.8495785	3.1334591	-3.4616731
C	-2.0441194	2.7454753	-4.5463932
C	-0.6747581	2.5134880	-4.3341407
C	-0.3967881	2.9798166	-0.5553651
C	0.7801419	2.4714631	-0.0491718
C	1.5976004	1.5015507	-0.8341550
C	1.1071812	0.2088938	-1.1198121
C	1.9100082	-0.7212022	-1.7928564
C	3.2131490	-0.3797339	-2.1939963
C	3.7080773	0.9066570	-1.9258372
C	2.9088850	1.8424344	-1.2478635
Br	-1.2150934	4.6507703	0.5665223
C	1.1254125	0.2657652	2.1664651
C	2.5789536	-0.1445763	2.1179675
C	0.1360492	-0.6351615	1.9919589
C	0.8133966	1.7248846	2.4184928
C	1.3007229	2.7630144	1.3707596
O	2.7084365	2.9522290	1.4083131
H	0.8770913	3.7399345	1.6751402
H	-0.2967372	1.8415113	2.5029275
H	1.2547380	2.0400824	3.3910045
H	-0.9200228	-0.3228909	1.9916986
H	0.3531452	-1.7003321	1.8153911
H	3.1663910	0.3213278	2.9362221
H	3.0477292	0.1617397	1.1548879
H	2.6943626	-1.2438234	2.1821984
H	3.1284741	2.1096156	1.1461889
H	0.0956552	-0.0591109	-0.7919562
H	1.5082974	-1.7232937	-1.9991073
H	3.8412442	-1.1155638	-2.7189712
H	4.7218232	1.1889771	-2.2489291
H	3.2835298	2.8565485	-1.0515488

H	-2.9310336	3.5478036	-1.3408785
H	-3.9232821	3.3301583	-3.6004569
H	-2.4774506	2.6380735	-5.5522537
H	-0.0240103	2.2352807	-5.1770496
H	0.9539528	2.4457129	-2.9152356
Pd	-1.8530482	2.1543931	0.7767512
P	-3.2672119	0.5336555	0.1076065
C	-4.0917325	-0.5170669	1.3800778
C	-4.6884045	1.1511756	-0.8999535
C	-2.4709545	-0.6991073	-1.0011198
C	-5.0393193	-1.5045963	1.0383016
C	-5.6365542	-2.2826445	2.0402230
C	-5.2941392	-2.0802829	3.3898770
C	-4.3557859	-1.0951405	3.7360441
C	-3.7586721	-0.3134247	2.7331207
H	-5.3108642	-1.6631547	-0.0162366
H	-6.3761310	-3.0512366	1.7684656
H	-5.7651306	-2.6924807	4.1739927
H	-4.0880736	-0.9309202	4.7907158
H	-3.0265806	0.4707347	2.9880271
C	-5.2359329	0.4432995	-1.9886989
C	-6.2948028	0.9945867	-2.7283886
C	-6.8210688	2.2502900	-2.3829585
C	-6.2873913	2.9546413	-1.2892809
C	-5.2235383	2.4100117	-0.5558837
H	-4.8196114	-0.5332648	-2.2764093
H	-6.7080854	0.4395960	-3.5844693
H	-7.6459609	2.6831154	-2.9691496
H	-6.6927664	3.9402885	-1.0147244
H	-4.7727004	2.9674915	0.2820028
C	-2.0594572	-1.9585417	-0.5172810
C	-1.3478327	-2.8374945	-1.3502848
C	-1.0427623	-2.4706994	-2.6714648
C	-1.4359867	-1.2092865	-3.1520812
C	-2.1388267	-0.3250647	-2.3235609
H	-2.3018388	-2.2554142	0.5134561
H	-1.0354191	-3.8193168	-0.9630292
H	-0.4921026	-3.1644198	-3.3247923
H	-1.1848667	-0.9003177	-4.1775751
H	-2.4268141	0.6639870	-2.7054372

R3

75

SCF Energy = -4548.289478861

C	0.5898813	5.7216184	-1.3895431
C	0.0544613	4.6394315	-0.6567231

C	-1.2147736	4.1419668	-1.0352551
C	-1.9113773	4.6883472	-2.1171463
C	-1.3663833	5.7611260	-2.8405173
C	-0.1138417	6.2744963	-2.4690746
C	0.7966134	3.9611885	0.4377392
C	1.1251077	2.6204475	0.4557197
C	0.6615439	1.7420949	-0.6558721
C	-0.0669032	0.5520293	-0.4100893
C	-0.4832744	-0.2747826	-1.4668997
C	-0.1825076	0.0681791	-2.7935581
C	0.5528416	1.2391060	-3.0529400
C	0.9745415	2.0592622	-2.0005528
Br	2.2325058	5.3153856	1.3521088
C	0.7080801	2.2032384	3.7360546
C	-0.5200698	1.6598104	4.4259277
C	1.3669334	3.3176826	4.1955620
C	1.3185943	1.2865019	2.6881102
C	2.0399501	1.9586719	1.4941961
O	2.9166641	1.0286282	0.8658663
H	2.6989116	2.7570760	1.8908503
H	2.0769244	0.6403033	3.1849920
H	0.5397764	0.5927549	2.3122611
H	2.3642187	3.6005499	3.8292257
H	0.9827756	3.8729793	5.0668101
H	-1.3485417	1.4777783	3.7122609
H	-0.8839983	2.3369058	5.2221415
H	-0.2806814	0.6802308	4.8969436
H	2.3597305	0.4385862	0.3187532
H	-0.3382339	0.2814482	0.6200379
H	-1.0561774	-1.1889929	-1.2478832
H	-0.5138743	-0.5752301	-3.6223968
H	0.8063095	1.5125374	-4.0884923
H	1.5569956	2.9675088	-2.2082382
H	-1.6562129	3.3097460	-0.4743268
H	-2.8983479	4.2830012	-2.3831284
H	-1.9212117	6.2014619	-3.6822975
H	0.3247035	7.1173764	-3.0247792
H	1.5714013	6.1243230	-1.1061779
Pd	0.0067040	4.3356766	2.4170860
P	-2.2093178	4.7989331	2.2928305
C	-2.8536286	5.8969065	0.9628846
C	-2.0126009	6.9538403	0.5573732
H	-1.0105581	7.0425534	1.0069367
C	-2.4371399	7.8514881	-0.4309810
H	-1.7707599	8.6664790	-0.7499052
C	-3.6982335	7.6932482	-1.0313562

H	-4.0253439	8.3905368	-1.8175684
C	-4.5333614	6.6347443	-0.6384135
H	-5.5175905	6.5025324	-1.1135011
C	-4.1150836	5.7379830	0.3577365
H	-4.7677398	4.9048108	0.6568617
C	-2.8670291	5.6157797	3.8122231
C	-2.5720317	5.0162064	5.0568274
H	-1.9771734	4.0906775	5.0792901
C	-3.0308624	5.5895486	6.2496441
H	-2.7991369	5.1085982	7.2122617
C	-3.7769105	6.7819274	6.2169651
H	-4.1304449	7.2382418	7.1539393
C	-4.0639686	7.3889563	4.9842968
H	-4.6456283	8.3229936	4.9515973
C	-3.6163208	6.8091277	3.7847781
H	-3.8504616	7.2858956	2.8220257
C	-3.2746990	3.2943802	2.1820646
C	-4.5884219	3.2467542	2.6924069
H	-5.0104068	4.1299789	3.1958477
C	-5.3499199	2.0726892	2.5718298
H	-6.3730705	2.0417138	2.9767494
C	-4.8097638	0.9398437	1.9387696
H	-5.4106565	0.0226075	1.8443372
C	-3.4968993	0.9775949	1.4384739
H	-3.0621371	0.0931994	0.9484492
C	-2.7305591	2.1448282	1.5715284
H	-1.6864577	2.1716314	1.2226991

R4

75

SCF Energy = -4548.298302432

C	2.9293950	1.3541867	-1.5684726
C	1.8146257	1.4417901	-0.7027362
C	1.2449034	0.2484512	-0.2050207
C	1.7603652	-1.0015353	-0.5785467
C	2.8614440	-1.0780155	-1.4475704
C	3.4449240	0.1017336	-1.9388052
C	1.2774027	2.7712214	-0.2929429
Pd	-1.2407137	3.6365003	0.9827891
P	-3.5303151	3.3912175	0.5962788
C	0.0397021	3.1436157	-0.7200193
Br	-0.3628336	5.3245685	-0.8082220
C	-0.7355412	2.4739001	-1.7906154
C	-0.6258239	2.9017187	-3.1330495
C	-1.3645690	2.2677996	-4.1417373
C	-2.2198861	1.1960448	-3.8269095

C	-2.3202851	0.7515162	-2.4990377
C	-1.5839783	1.3871575	-1.4895887
C	2.0987366	3.5512608	0.7276434
O	3.4963493	3.4014686	0.5301364
C	1.6721652	3.1306842	2.1592902
C	0.3362755	3.6921572	2.6033930
C	-0.7360807	2.8433457	2.9419811
C	0.3693193	5.1317860	3.0875131
H	1.8894467	4.6318494	0.5891258
H	2.4729915	3.4887923	2.8435970
H	1.6676969	2.0206521	2.2139143
H	-0.5993181	1.7495255	2.9038482
H	-1.5469025	3.1979896	3.6012284
H	1.0020354	5.2205332	3.9998637
H	-0.6430033	5.5047492	3.3372126
H	0.8014470	5.8118248	2.3252688
H	3.6929719	2.4442253	0.5805334
H	0.3874132	0.3163740	0.4799480
H	1.2991196	-1.9215158	-0.1882354
H	3.2650392	-2.0583368	-1.7431682
H	4.3052599	0.0477657	-2.6233641
H	3.3765885	2.2805844	-1.9558091
H	-1.6774600	1.0573300	-0.4480414
H	-2.9871661	-0.0821169	-2.2358098
H	-2.8089037	0.7095264	-4.6190619
H	-1.2757535	2.6153064	-5.1822632
H	0.0297416	3.7522624	-3.3684373
C	-4.4002967	4.2613302	-0.7728029
C	-4.3748202	4.0612199	2.0935449
C	-4.2016938	1.6801278	0.4797099
C	-5.1531695	1.2917148	-0.4827985
C	-5.5639942	-0.0496312	-0.5676860
C	-5.0342897	-1.0101837	0.3087009
C	-4.0887871	-0.6252680	1.2775374
C	-3.6694245	0.7095534	1.3575930
H	-5.5641612	2.0399727	-1.1757205
H	-6.3031207	-0.3448287	-1.3281575
H	-5.3552646	-2.0604978	0.2375897
H	-3.6688348	-1.3734570	1.9670730
H	-2.9081873	1.0127948	2.0935028
C	-5.6431256	4.9049600	-0.5982590
C	-6.2704889	5.5308702	-1.6872788
C	-5.6660438	5.5150694	-2.9560701
C	-4.4263629	4.8772519	-3.1318394
C	-3.7905607	4.2604867	-2.0447163
H	-6.1203775	4.9148413	0.3930130

H	-7.2392070	6.0336485	-1.5434304
H	-6.1604842	6.0068456	-3.8077876
H	-3.9409544	4.8652068	-4.1193746
H	-2.8156512	3.7759602	-2.1819147
C	-5.4117464	3.3905461	2.7710758
C	-5.9795756	3.9544998	3.9267622
C	-5.5257423	5.1934744	4.4067005
C	-4.4956720	5.8710141	3.7291433
C	-3.9175116	5.3046650	2.5847318
H	-5.7736610	2.4223699	2.3946861
H	-6.7853398	3.4206479	4.4536499
H	-5.9719412	5.6317477	5.3122847
H	-4.1342285	6.8418007	4.1010728
H	-3.0957363	5.8197748	2.0605189

S1

75

SCF Energy = -4548.290184978

C	-0.4540655	2.8039101	-2.4599764
C	-0.7702249	3.0166202	-1.0929274
C	-2.0323300	3.5864127	-0.7956342
C	-2.9686133	3.8630088	-1.7968645
C	-2.6648560	3.5856988	-3.1409170
C	-1.3970589	3.0703632	-3.4621059
C	0.1731775	2.6730505	-0.0094466
C	1.4184969	2.0874097	-0.0630211
C	1.7346626	1.1459010	-1.1727352
C	0.8932432	0.0415430	-1.4394878
C	1.2174036	-0.8660217	-2.4574203
C	2.3831657	-0.6901513	-3.2216382
C	3.2335734	0.3971950	-2.9532087
C	2.9190945	1.3060491	-1.9329043
Br	0.1004671	4.5222324	1.4998380
C	1.5140811	1.4379353	3.0941849
C	1.2328164	1.7781483	4.5420278
C	1.0440756	0.2725068	2.5359037
C	2.4561727	2.3935583	2.4030668
C	2.6248568	2.3299398	0.8695296
O	3.3046069	3.5074065	0.4209770
H	3.3250961	1.5003934	0.6475641
H	2.1638049	3.4280533	2.6736742
H	3.4771269	2.2640978	2.8309388
H	1.3453949	-0.0644593	1.5331570
H	0.4704871	-0.4451384	3.1430009
H	0.8144294	2.8012848	4.6398025
H	2.1744536	1.7607765	5.1340179

H	0.5281252	1.0614376	5.0070997
H	2.6507443	4.2319174	0.5335493
H	-0.0168801	-0.0954059	-0.8391937
H	0.5499023	-1.7187861	-2.6466940
H	2.6337769	-1.4037231	-4.0213083
H	4.1495618	0.5412595	-3.5467633
H	3.5681004	2.1692979	-1.7225074
H	-2.2675229	3.8179881	0.2478513
H	-3.9446350	4.2860321	-1.5153661
H	-3.4012511	3.7872150	-3.9334726
H	-1.1294143	2.8754141	-4.5117817
H	0.5288620	2.4102670	-2.7407969
Pd	-0.6482890	1.9793074	1.7725777
P	-2.6565934	0.9629961	1.3472961
C	-4.1765515	1.9623084	1.0270792
C	-4.2684576	3.2055873	1.6867409
H	-3.4330968	3.5338646	2.3278499
C	-5.3908764	4.0256239	1.5029589
H	-5.4488202	4.9966333	2.0175654
C	-6.4299960	3.6138744	0.6498758
H	-7.3054078	4.2622987	0.4934711
C	-6.3460465	2.3739488	-0.0051589
H	-7.1575104	2.0470802	-0.6732987
C	-5.2270040	1.5471998	0.1852783
H	-5.1649398	0.5825965	-0.3393081
C	-2.5726229	-0.2107190	-0.0640730
C	-2.1806449	-1.5494023	0.1580200
H	-2.0322245	-1.9119854	1.1859917
C	-1.9807260	-2.4186626	-0.9250843
H	-1.6815061	-3.4610372	-0.7372599
C	-2.1617973	-1.9623203	-2.2420940
H	-2.0096744	-2.6466333	-3.0904793
C	-2.5279024	-0.6254795	-2.4694110
H	-2.6504762	-0.2485786	-3.4956260
C	-2.7299844	0.2481141	-1.3911858
H	-3.0048791	1.2931431	-1.5862781
C	-3.2342900	-0.1027986	2.7441344
C	-2.5517235	-0.0260369	3.9730495
H	-1.6866205	0.6523974	4.0582722
C	-2.9705033	-0.7974792	5.0697800
H	-2.4312009	-0.7286678	6.0266918
C	-4.0750860	-1.6542245	4.9409895
H	-4.4043051	-2.2623210	5.7972652
C	-4.7637136	-1.7329920	3.7166275
H	-5.6325370	-2.4011708	3.6151865
C	-4.3492552	-0.9582364	2.6239313

H	-4.8931186	-1.0199379	1.6692923
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S2

75

SCF Energy = -4548.290721847

C	-0.0538966	4.6729997	-1.4737749
C	-0.5308518	3.5335728	-0.7806584
C	-1.7560904	2.9548155	-1.1823698
C	-2.4802468	3.4878515	-2.2546784
C	-2.0040217	4.6253240	-2.9251243
C	-0.7886464	5.2158853	-2.5321542
C	0.2959656	2.9556443	0.2849766
C	1.5340821	2.3811448	0.1244947
C	1.8163928	1.7861313	-1.2146597
C	0.9090222	0.8905008	-1.8228179
C	1.1807963	0.3419268	-3.0842637
C	2.3674121	0.6755902	-3.7576581
C	3.2824747	1.5574572	-3.1563151
C	3.0166773	2.1065461	-1.8941624
Br	0.6799931	4.9927339	1.9832249
C	1.4944093	1.0479035	2.8426524
C	1.6339189	-0.2760801	2.1260243
C	0.5690807	1.2277823	3.8479248
C	2.5332068	2.1112579	2.5656510
C	2.7608193	2.4142230	1.0664508
O	3.4437429	3.6448749	0.8869916
H	3.4469596	1.6403852	0.6663797
H	2.2454931	3.0507272	3.0747768
H	3.5145826	1.7987101	2.9893252
H	0.5915560	2.1252282	4.4869207
H	-0.1038000	0.4071509	4.1460612
H	2.5766007	-0.7741963	2.4444478
H	1.6915945	-0.1545266	1.0262638
H	0.7910941	-0.9563512	2.3545902
H	2.7981992	4.3362413	1.1854679
H	-0.0097808	0.6176278	-1.2831071
H	0.4632276	-0.3564425	-3.5414567
H	2.5815841	0.2462724	-4.7481448
H	4.2126101	1.8274709	-3.6797769
H	3.7148301	2.8177302	-1.4280190
H	-2.1260306	2.0704847	-0.6453095
H	-3.4309427	3.0244904	-2.5551379
H	-2.5830007	5.0564531	-3.7557224
H	-0.4131616	6.1067337	-3.0579119
H	0.8928771	5.1254278	-1.1468452
Pd	-0.5191576	2.2957172	1.9793169

P	-2.7249887	2.9491768	2.1574202
C	-3.4872372	4.1680544	1.0133147
C	-2.7461885	5.3333985	0.7144403
H	-1.7537221	5.4836514	1.1704677
C	-3.2564544	6.2747629	-0.1886806
H	-2.6660782	7.1728608	-0.4229605
C	-4.4999544	6.0615959	-0.8082870
H	-4.8926076	6.7975769	-1.5263075
C	-5.2353549	4.9018323	-0.5166240
H	-6.2076558	4.7270158	-1.0023022
C	-4.7339286	3.9560643	0.3921762
H	-5.3103694	3.0451171	0.6074061
C	-3.9065816	1.5354841	2.1431783
C	-5.1533437	1.5938420	2.8013393
H	-5.4310766	2.4984538	3.3634154
C	-6.0299088	0.4995379	2.7446385
H	-6.9995924	0.5484814	3.2632282
C	-5.6711666	-0.6574256	2.0304382
H	-6.3603074	-1.5146792	1.9901959
C	-4.4279673	-0.7231123	1.3792603
H	-4.1384377	-1.6318784	0.8301204
C	-3.5456535	0.3669506	1.4428366
H	-2.5503994	0.3191420	0.9696939
C	-3.0181836	3.6819218	3.8233118
C	-2.6892960	2.8906620	4.9466504
H	-2.3052343	1.8693006	4.7976357
C	-2.8506394	3.3976689	6.2421928
H	-2.5961049	2.7706390	7.1102475
C	-3.3271217	4.7078080	6.4320257
H	-3.4440278	5.1106257	7.4494360
C	-3.6494009	5.4992449	5.3188980
H	-4.0227299	6.5249532	5.4603351
C	-3.5012017	4.9898200	4.0174815
H	-3.7603520	5.6133480	3.1500410

S3

75

SCF Energy = -4548.294596929

C	0.1379066	5.2386099	-1.4819728
C	-0.5950684	4.3489817	-0.6602248
C	-1.8788951	3.9305676	-1.0866065
C	-2.4085258	4.3685222	-2.3056860
C	-1.6706009	5.2497317	-3.1117875
C	-0.3966751	5.6810179	-2.6963599
C	-0.0125574	3.8131480	0.5739167
C	1.0547834	2.9459484	0.7103415

C	1.5783682	2.2177917	-0.4792561
C	0.7122386	1.6633417	-1.4535422
C	1.2164239	0.9871110	-2.5716899
C	2.6025339	0.8359404	-2.7456741
C	3.4762263	1.3733157	-1.7867850
C	2.9731639	2.0533351	-0.6678747
Br	0.7047013	6.0891020	1.7423273
C	0.1328127	0.7678628	2.5375215
C	-0.3583576	-0.2062708	1.4974533
C	-0.6706184	1.1925676	3.5653122
C	1.6012367	1.1763242	2.4481294
C	1.7821748	2.6586472	2.0471461
O	1.3358944	3.4322394	3.1337440
H	2.8738608	2.8332912	1.8773011
H	2.1032219	1.0371120	3.4278427
H	2.1230740	0.5372483	1.7094895
H	-0.2642617	1.7878067	4.3957172
H	-1.7025493	0.8138329	3.6625608
H	-0.1168271	0.1422038	0.4730041
H	-1.4489442	-0.3824056	1.5723639
H	0.1628592	-1.1812995	1.6226975
H	1.2663270	4.3863081	2.8313945
H	-0.3732879	1.7658665	-1.3236732
H	0.5172089	0.5684535	-3.3115151
H	2.9990904	0.3021587	-3.6223841
H	4.5650412	1.2711317	-1.9129783
H	3.6773089	2.4870848	0.0562756
H	-2.4447617	3.2459235	-0.4373799
H	-3.4092986	4.0360211	-2.6168509
H	-2.0908908	5.6095690	-4.0632681
H	0.1822274	6.3734371	-3.3262060
H	1.1195817	5.5864242	-1.1318168
Pd	-1.1512315	3.0566343	2.0493853
P	-2.8207686	4.5138957	2.4232773
C	-3.4892938	5.5178952	1.0426226
C	-2.6726578	6.5426336	0.5119814
H	-1.6891934	6.7476910	0.9656567
C	-3.1023075	7.2693178	-0.6052419
H	-2.4545177	8.0568552	-1.0178010
C	-4.3388152	6.9805133	-1.2074085
H	-4.6690948	7.5484057	-2.0904633
C	-5.1515500	5.9628673	-0.6816930
H	-6.1239556	5.7367589	-1.1455402
C	-4.7310504	5.2309601	0.4403969
H	-5.3720347	4.4362301	0.8497472
C	-2.4367448	5.7478508	3.7206687

C	-1.3817141	5.4690427	4.6118431
H	-0.7881594	4.5528286	4.4687706
C	-1.0707525	6.3754976	5.6351206
H	-0.2378401	6.1591902	6.3206316
C	-1.8030694	7.5674997	5.7657295
H	-1.5503073	8.2843558	6.5618341
C	-2.8477136	7.8541435	4.8703542
H	-3.4139268	8.7933040	4.9642398
C	-3.1657704	6.9479137	3.8467905
H	-3.9717165	7.1783072	3.1337719
C	-4.2884981	3.5958835	3.0553141
C	-5.1042801	4.0729650	4.1005150
H	-4.8768904	5.0390046	4.5748305
C	-6.1987987	3.3115211	4.5413527
H	-6.8275543	3.6876293	5.3627970
C	-6.4917937	2.0757723	3.9406967
H	-7.3502046	1.4824045	4.2903771
C	-5.6800795	1.5938616	2.8989344
H	-5.9003906	0.6229284	2.4296894
C	-4.5778481	2.3451930	2.4657644
H	-3.9173524	1.9643770	1.6687005

S4

75

SCF Energy = -4548.294788801

C	-0.8373856	3.9707246	-2.1511630
C	-1.0481673	3.0520576	-1.0956414
C	-1.9195216	1.9580862	-1.3110249
C	-2.5506885	1.7746926	-2.5467783
C	-2.3339773	2.6936421	-3.5855340
C	-1.4737669	3.7893180	-3.3838322
C	-0.3378019	3.1977911	0.1820492
C	1.0075390	3.0215259	0.4368051
C	1.8628717	2.3586458	-0.5881143
C	1.4616898	1.1532337	-1.2111250
C	2.2691362	0.5344413	-2.1747773
C	3.5048972	1.0991942	-2.5324509
C	3.9213009	2.2913747	-1.9175098
C	3.1116627	2.9146561	-0.9562896
Br	-0.9654707	5.6196974	0.7912710
C	1.1493865	1.3549757	3.1255082
C	0.8413541	1.6617727	4.5703198
C	0.4902355	0.3704365	2.4318629
C	2.2628870	2.1621559	2.4817247
C	1.7281722	3.4227010	1.7371055
O	0.9430025	4.1349363	2.6622723

H	2.6235862	4.0235580	1.4363925
H	2.9675237	2.5105390	3.2636303
H	2.8331607	1.5449030	1.7604590
H	0.8244242	0.0633237	1.4284861
H	-0.2530499	-0.2703035	2.9355787
H	0.6930212	2.7516226	4.7024152
H	1.7043779	1.3739947	5.2104761
H	-0.0558023	1.1223407	4.9314885
H	0.4030673	4.8167766	2.1669742
H	0.4993865	0.7036299	-0.9292071
H	1.9316293	-0.4011345	-2.6463617
H	4.1409662	0.6125082	-3.2871220
H	4.8831047	2.7490808	-2.1957258
H	3.4404878	3.8618270	-0.5041936
H	-2.0857002	1.2543274	-0.4814595
H	-3.2295179	0.9217396	-2.6909556
H	-2.8410734	2.5620866	-4.5535636
H	-1.3022069	4.5112314	-4.1966990
H	-0.1833627	4.8354564	-1.9724298
Pd	-0.9796641	2.2262153	1.8376260
P	-3.1668074	2.6954613	2.1243612
C	-3.4819442	4.2091562	3.1028042
C	-2.4463012	4.6849434	3.9315463
H	-1.4709186	4.1733667	3.9176883
C	-2.6490956	5.8250307	4.7215278
H	-1.8336108	6.1998258	5.3579210
C	-3.8803348	6.5008909	4.6779848
H	-4.0346794	7.4032051	5.2891615
C	-4.9101911	6.0360034	3.8422567
H	-5.8706909	6.5717449	3.7990357
C	-4.7141706	4.8915061	3.0534826
H	-5.5133255	4.5332740	2.3871327
C	-3.9713047	1.3399657	3.0794297
C	-4.9089437	1.5721899	4.1053697
H	-5.1958225	2.6027602	4.3610047
C	-5.4684564	0.4903230	4.8045039
H	-6.1953814	0.6801099	5.6089600
C	-5.1050812	-0.8278298	4.4818440
H	-5.5462991	-1.6721910	5.0328225
C	-4.1693986	-1.0655705	3.4597955
H	-3.8759567	-2.0957263	3.2066453
C	-3.5973364	0.0131825	2.7697996
H	-2.8431960	-0.1610250	1.9843897
C	-4.2258112	2.8760133	0.6372253
C	-5.1096561	1.8596417	0.2209237
H	-5.2556395	0.9656820	0.8448231

C	-5.8068799	1.9889391	-0.9910968
H	-6.4973383	1.1924413	-1.3084739
C	-5.6289708	3.1288894	-1.7920144
H	-6.1724098	3.2238031	-2.7443296
C	-4.7528014	4.1452172	-1.3752445
H	-4.5978314	5.0361233	-2.0016006
C	-4.0490059	4.0224815	-0.1706560
H	-3.3370027	4.8040036	0.1386735

Optimized Geometries(MXn)(TS_ab)

R1
75
SCF Energy = -4548.276110082

C	0.9072926	3.2294051	-3.0262411
C	0.1280717	3.5860169	-1.8985236
C	-1.2764796	3.6254894	-2.0304096
C	-1.8868206	3.3046327	-3.2526328
C	-1.1063916	2.9427854	-4.3623156
C	0.2942459	2.9082193	-4.2412385
C	0.8199189	3.8757248	-0.6177513
C	1.7354147	3.0822528	0.0343219
C	2.2104897	1.8531176	-0.6635692
C	1.3267229	0.8107787	-1.0243108
C	1.7803906	-0.2940105	-1.7555907
C	3.1263356	-0.3777671	-2.1513371
C	4.0115862	0.6583110	-1.8133123
C	3.5613623	1.7640218	-1.0778348
Br	-0.1236283	5.3714741	0.4746762
C	1.2536556	1.4213432	2.5606476
C	-0.0958065	0.9667647	2.0692992
C	2.2253897	0.5555274	2.9283821
C	1.4736052	2.9170004	2.5971234
C	2.3335015	3.4332477	1.4077194
O	3.6746697	2.9918413	1.5343401
H	2.3777830	4.5381181	1.4931828
H	0.5059138	3.4573957	2.5878265
H	2.0175445	3.2200056	3.5151120
H	3.1767337	0.9097419	3.3567132
H	2.0857132	-0.5339207	2.8459981
H	-0.3957111	1.5231440	1.1573922
H	-0.8705070	1.1954622	2.8341779
H	-0.1277379	-0.1188508	1.8560682
H	3.6567508	2.0130255	1.4606033

H	0.2668754	0.8842096	-0.7476027
H	1.0734088	-1.0924062	-2.0277878
H	3.4800816	-1.2421178	-2.7335537
H	5.0596732	0.6232194	-2.1450192
H	4.2434703	2.5954260	-0.8603950
H	-1.8901215	3.9153720	-1.1657637
H	-2.9836569	3.3398616	-3.3364111
H	-1.5873852	2.6940087	-5.3204011
H	0.9211762	2.6309304	-5.1021061
H	2.0001045	3.2014196	-2.9377265
Pd	1.9931006	5.6847815	-0.9778479
P	3.9370926	6.1687301	-1.9982435
C	4.0524341	7.6418188	-3.0985804
C	4.9724120	7.7190385	-4.1653569
H	5.6339255	6.8659993	-4.3798642
C	5.0383383	8.8782435	-4.9540889
H	5.7548346	8.9320015	-5.7881166
C	4.1917115	9.9667537	-4.6813362
H	4.2434751	10.8733217	-5.3034711
C	3.2729236	9.8926654	-3.6206001
H	2.6024683	10.7397337	-3.4100968
C	3.1983850	8.7315745	-2.8357484
H	2.4676381	8.6465456	-2.0145287
C	5.3600754	6.3725283	-0.8435265
C	5.4351039	5.4907267	0.2575166
H	4.6578687	4.7272030	0.4193498
C	6.5069103	5.5765942	1.1574473
H	6.5514967	4.8772579	2.0059931
C	7.5004267	6.5562080	0.9831667
H	8.3342297	6.6322210	1.6978053
C	7.4203114	7.4441995	-0.1019373
H	8.1909460	8.2181261	-0.2401548
C	6.3583014	7.3517235	-1.0172506
H	6.3038588	8.0483920	-1.8665915
C	4.5113615	4.8120512	-3.1119831
C	3.7245374	4.5151287	-4.2470885
H	2.8242282	5.1138158	-4.4554933
C	4.0806188	3.4616491	-5.0999289
H	3.4619249	3.2422164	-5.9834888
C	5.2206320	2.6845839	-4.8264306
H	5.4933227	1.8509728	-5.4908403
C	6.0100884	2.9813044	-3.7046916
H	6.9108237	2.3857979	-3.4901767
C	5.6611611	4.0413829	-2.8506425
H	6.2864938	4.2712907	-1.9759472

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R2
75
SCF Energy = -4548.277431785
C      1.6518852      3.4290272     -2.8378573
C      0.4997957      3.7361724     -2.0666059
C     -0.7438312      3.8272698     -2.7279173
C     -0.8364997      3.6156819     -4.1131126
C      0.3078269      3.3048204     -4.8633489
C      1.5521420      3.2122429     -4.2141974
C      0.6603103      3.9911584     -0.6105699
C      1.4292465      3.2786301      0.2867339
C      2.1906401      2.0990443     -0.2089821
C      1.5193369      0.9850091     -0.7622369
C      2.2406906     -0.1211024     -1.2267831
C      3.6454559     -0.1356946     -1.1506842
C      4.3227696      0.9720095     -0.6177847
C      3.6037669      2.0842577     -0.1515868
Br    -0.7614881      5.2570613      0.1680825
C      0.3207227      1.2936886      2.3541775
C      1.5058711      0.4582284      2.7750399
C     -0.7763469      0.7355010      1.7993979
C      0.3947969      2.7873896      2.5762318
C      1.4860821      3.5712844      1.7935244
O      2.7857128      3.3948048      2.3385840
H      1.2610321      4.6457109      1.9445757
H     -0.5835918      3.2416320      2.3206937
H      0.5880865      3.0021159      3.6509994
H     -1.6334837      1.3517531      1.4847790
H     -0.8501941     -0.3521338      1.6391872
H      1.8515093      0.7279771      3.7948079
H      2.3673666      0.6083030      2.0865936
H      1.2718030     -0.6236550      2.7543143
H      3.0726461      2.4836740      2.1305090
H      0.4224122      0.9981660     -0.8140985
H      1.7027283     -0.9816574     -1.6528586
H      4.2098057     -1.0063894     -1.5177533
H      5.4218634      0.9870213     -0.5804285
H      4.1337610      2.9750655      0.2117005
H     -1.6428520      4.0804105     -2.1492255
H     -1.8166918      3.6967079     -4.6070586
H      0.2345468      3.1458751     -5.9496485
H      2.4625988      2.9878069     -4.7897373
H      2.6337065      3.3894697     -2.3509614
Pd     1.7246171      5.8627794     -0.5536918
P      3.4530867      6.6954510     -1.7046898
C      4.3971107      8.1891750     -1.1742147

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C	5.7817270	8.3498129	-1.3914593
H	6.3614770	7.5407996	-1.8608818
C	6.4240666	9.5342294	-0.9962588
H	7.5055273	9.6511657	-1.1656297
C	5.6911039	10.5660016	-0.3860890
H	6.1978544	11.4922016	-0.0749256
C	4.3121263	10.4086971	-0.1642461
H	3.7359459	11.2103725	0.3223110
C	3.6692061	9.2228562	-0.5495288
H	2.5925999	9.0777852	-0.3625338
C	4.7685393	5.4086218	-1.8374474
C	4.9432037	4.6338948	-3.0019309
H	4.3406155	4.8519235	-3.8956934
C	5.8843193	3.5907511	-3.0234522
H	6.0067983	2.9876216	-3.9359408
C	6.6730364	3.3248130	-1.8934707
H	7.4191511	2.5162376	-1.9180498
C	6.5033994	4.0954312	-0.7284626
H	7.1129055	3.8890207	0.1645982
C	5.5475374	5.1197732	-0.6942075
H	5.3976360	5.7020587	0.2282325
C	3.0531788	7.0573748	-3.4705834
C	1.7998090	6.6497038	-3.9690160
H	1.0830914	6.1707182	-3.2833515
C	1.4764771	6.8514166	-5.3200794
H	0.4981950	6.5188617	-5.6976235
C	2.3977444	7.4733387	-6.1779223
H	2.1436185	7.6367571	-7.2365100
C	3.6444699	7.8958046	-5.6817653
H	4.3650560	8.3918497	-6.3499637
C	3.9730965	7.6886352	-4.3338145
H	4.9483568	8.0230944	-3.9494213

R3

75

SCF Energy = -4548.274603258

C	1.7371565	4.5683459	-3.1201044
C	1.2846232	4.6912355	-1.7875066
C	-0.0515252	5.0847724	-1.5580093
C	-0.9124622	5.3386735	-2.6366341
C	-0.4520261	5.2120364	-3.9576539
C	0.8789623	4.8266036	-4.1938502
C	2.2104352	4.3628071	-0.6719776
C	2.8193030	3.1491391	-0.4436510
C	2.8035901	2.1364958	-1.5378086
C	1.6143785	1.5046925	-1.9638976

C	1.6335362	0.5896624	-3.0256404
C	2.8406567	0.2816423	-3.6772773
C	4.0307627	0.8997327	-3.2607303
C	4.0146951	1.8236281	-2.2032724
Br	1.9929059	5.6585332	0.9272483
C	1.4033019	2.2748013	2.2743817
C	0.1645911	2.2855280	1.4152265
C	1.3960053	2.7449372	3.5394044
C	2.6784412	1.7270316	1.6641872
C	3.5211342	2.7506162	0.8510242
O	4.8301436	2.2281614	0.6365196
H	3.6623519	3.6546976	1.4728928
H	3.3540842	1.3646364	2.4648550
H	2.4529351	0.8593746	1.0038388
H	2.3042385	2.7289470	4.1630142
H	0.4848257	3.1694011	3.9898951
H	-0.0744996	1.2619625	1.0537846
H	0.3111388	2.9114896	0.5105676
H	-0.7137899	2.6754897	1.9642674
H	4.7449785	1.4732982	0.0190138
H	0.6671813	1.7532894	-1.4658470
H	0.6953639	0.1144374	-3.3502511
H	2.8510001	-0.4355824	-4.5119182
H	4.9805531	0.6789632	-3.7715665
H	4.9343876	2.3542321	-1.9171950
H	-0.4107355	5.1993527	-0.5253588
H	-1.9515611	5.6438096	-2.4402896
H	-1.1270945	5.4221996	-4.8011398
H	1.2662907	4.7376364	-5.2197134
H	2.7759202	4.2778475	-3.3077752
Pd	3.9084790	5.7148942	-0.8088537
P	5.5490316	5.8524125	-2.3474250
C	6.5468802	7.4084040	-2.3513367
C	5.9783138	8.5441003	-1.7394500
H	4.9954844	8.4411987	-1.2482931
C	6.6610386	9.7711726	-1.7496638
H	6.2081088	10.6532835	-1.2720446
C	7.9244231	9.8661983	-2.3556785
H	8.4659134	10.8245120	-2.3556526
C	8.5021052	8.7322844	-2.9536756
H	9.4962016	8.8016622	-3.4213074
C	7.8165119	7.5082044	-2.9558231
H	8.2774567	6.6248874	-3.4211925
C	6.7987472	4.4993856	-2.2705678
C	6.9519070	3.8354999	-1.0367233
H	6.3081762	4.1175760	-0.1899534

C	7.8698188	2.7815436	-0.9070603
H	7.9603210	2.2617889	0.0582790
C	8.6429360	2.3825358	-2.0094077
H	9.3571939	1.5505722	-1.9118146
C	8.4946400	3.0395348	-3.2441427
H	9.0938727	2.7248928	-4.1123323
C	7.5768901	4.0929214	-3.3769514
H	7.4469591	4.5848216	-4.3525856
C	4.9583455	5.7636345	-4.0927907
C	4.6331866	6.9405000	-4.7978375
H	4.8314757	7.9220577	-4.3417143
C	4.0575651	6.8650828	-6.0755718
H	3.8088819	7.7918998	-6.6146310
C	3.8011072	5.6163854	-6.6666518
H	3.3513510	5.5606399	-7.6695249
C	4.1222642	4.4393323	-5.9688988
H	3.9210217	3.4544810	-6.4173151
C	4.6928549	4.5108245	-4.6895510
H	4.9244362	3.5829485	-4.1473538

R4

75

SCF Energy = -4548.277808098

C	1.0713160	5.3728791	-2.6082947
C	0.6323202	4.6092286	-1.5081177
C	-0.6684570	4.0550822	-1.5278606
C	-1.4887815	4.2182264	-2.6523110
C	-1.0244366	4.9439928	-3.7642140
C	0.2541956	5.5254240	-3.7367664
C	1.4900637	4.3893623	-0.3208022
C	2.0175894	3.1938381	0.1155574
C	2.1827137	2.0777233	-0.8666692
C	1.1048794	1.3437941	-1.4094184
C	1.3332289	0.2991540	-2.3176541
C	2.6422459	-0.0435129	-2.6979558
C	3.7244661	0.6733578	-2.1647046
C	3.4974469	1.7241624	-1.2617001
Br	1.1374854	5.9121030	1.0870552
C	0.1688354	2.3427187	2.4658114
C	-0.0066522	3.3354279	3.5873549
C	-0.8725345	1.9021001	1.7277045
C	1.5802279	1.8602969	2.2148336
C	2.5036523	2.9114029	1.5364353
O	3.8616339	2.4892771	1.6077348
H	2.4628901	3.8566392	2.1100946
H	2.0739385	1.5994078	3.1757848

H	1.5709008	0.9443041	1.5867239
H	-0.7335367	1.1493511	0.9363033
H	-1.8973597	2.2646072	1.9066048
H	0.6411329	4.2254505	3.4451504
H	0.2862421	2.8796100	4.5582627
H	-1.0533780	3.6860816	3.6692809
H	3.9577310	1.7144195	1.0165591
H	0.0789003	1.5981771	-1.1184425
H	0.4767616	-0.2550053	-2.7312003
H	2.8154435	-0.8632131	-3.4115990
H	4.7571965	0.4385108	-2.4628852
H	4.3439148	2.3190846	-0.8946095
H	-1.0239965	3.5094686	-0.6404446
H	-2.4976220	3.7781650	-2.6625950
H	-1.6673414	5.0667636	-4.6493007
H	0.6241449	6.1000987	-4.5988684
H	2.0672416	5.8368027	-2.5602092
Pd	3.3247948	5.5333950	-0.2490103
P	5.1244032	5.4819255	-1.5996811
C	6.3406778	6.8667930	-1.5984724
C	7.6842603	6.6963837	-1.9900606
H	8.0462647	5.7005353	-2.2872699
C	8.5585190	7.7943272	-1.9934788
H	9.6087188	7.6559371	-2.2923854
C	8.0966716	9.0668283	-1.6140957
H	8.7859620	9.9249541	-1.6149579
C	6.7581899	9.2398155	-1.2228659
H	6.3961201	10.2330725	-0.9168058
C	5.8846202	8.1413805	-1.2055502
H	4.8376545	8.2508916	-0.8767387
C	6.1820637	3.9927971	-1.3426166
C	6.4114588	3.5896029	-0.0094821
H	5.9577781	4.1630449	0.8129108
C	7.1551764	2.4318442	0.2599313
H	7.3145089	2.1192516	1.3028115
C	7.6668136	1.6601734	-0.7982248
H	8.2351761	0.7415851	-0.5868386
C	7.4445416	2.0597127	-2.1270391
H	7.8439090	1.4584966	-2.9582610
C	6.7091790	3.2248736	-2.4012650
H	6.5244715	3.5275049	-3.4425122
C	4.6455328	5.3482251	-3.3739507
C	3.8539014	4.2432490	-3.7628374
H	3.5846901	3.4745933	-3.0238501
C	3.3952992	4.1303085	-5.0809612
H	2.7789481	3.2647098	-5.3658436

C	3.7005602	5.1286156	-6.0235585
H	3.3296841	5.0457162	-7.0564960
C	4.4769382	6.2341194	-5.6396022
H	4.7178622	7.0198326	-6.3718955
C	4.9545412	6.3437004	-4.3220957
H	5.5675900	7.2088293	-4.0291957

S1

75

SCF Energy = -4548.277294829

C	2.6939437	4.7918292	-2.5016794
C	1.6021984	4.4331782	-1.6854918
C	0.3949669	4.0224424	-2.2954517
C	0.2996623	3.9357227	-3.6909593
C	1.4072218	4.2590729	-4.4960992
C	2.6016912	4.6904605	-3.8970423
C	1.7261370	4.4327067	-0.2040378
C	2.1899852	3.4227623	0.6252658
C	3.0387219	2.3386812	0.0509432
C	2.7858750	1.7157965	-1.1952795
C	3.6652374	0.7563116	-1.7149354
C	4.8244735	0.3892684	-1.0111955
C	5.0858962	0.9893218	0.2319822
C	4.2063651	1.9447478	0.7556759
Br	0.3409634	5.8190994	0.5673159
C	0.4319514	1.2397522	1.7020343
C	-0.3324407	1.1876892	0.4058623
C	1.0300846	0.1545892	2.2344144
C	0.5356202	2.5974773	2.3718538
C	1.9003731	3.3048230	2.1343174
O	1.9925043	4.4869974	2.9107758
H	2.6792104	2.6368837	2.5478610
H	-0.2717975	3.2704090	2.0140863
H	0.4255620	2.5061444	3.4715934
H	1.5808817	0.2115088	3.1873404
H	1.0000126	-0.8243663	1.7313064
H	0.0686532	1.9302513	-0.3149293
H	-1.3992842	1.4563535	0.5680161
H	-0.2896343	0.1876913	-0.0664336
H	1.3139978	5.1139249	2.5786397
H	1.8882802	1.9770947	-1.7671770
H	3.4365651	0.2890602	-2.6849648
H	5.5156270	-0.3596609	-1.4263275
H	5.9923893	0.7300048	0.7989865
H	4.4588269	2.4289048	1.7078286
H	-0.4698197	3.7719700	-1.6632435

H	-0.6441586	3.6103906	-4.1542053
H	1.3321870	4.1839883	-5.5916377
H	3.4745946	4.9543811	-4.5125670
H	3.6208734	5.1331358	-2.0261616
C	5.5257813	8.8632025	0.6145703
C	6.1995386	7.6461350	0.8399840
C	7.5364419	7.6617639	1.2874575
C	8.1916225	8.8844501	1.4981763
C	7.5209676	10.0967343	1.2577964
C	6.1882107	10.0851189	0.8138955
P	5.2812480	6.0840768	0.4985231
C	5.9823534	5.5449692	-1.1175259
C	6.5392017	6.4655516	-2.0284000
C	6.9290003	6.0415360	-3.3097346
C	6.7744378	4.6979572	-3.6915218
C	6.2252744	3.7752830	-2.7835403
C	5.8250316	4.1949038	-1.5079557
Pd	3.0225954	5.9613655	0.5135375
C	5.9931354	4.8664653	1.6873787
C	7.1777405	4.1438201	1.4356939
C	7.6306597	3.1884250	2.3598627
C	6.9117584	2.9547053	3.5446587
C	5.7357116	3.6802627	3.8035540
C	5.2729512	4.6275936	2.8773005
H	7.7331241	4.3077265	0.5003783
H	8.5492973	2.6193257	2.1500544
H	7.2649267	2.1994611	4.2633048
H	5.1589877	3.4935750	4.7220523
H	4.3124721	5.1411468	3.0435631
H	6.6651482	7.5184079	-1.7349824
H	7.3608263	6.7690749	-4.0140330
H	7.0822451	4.3702648	-4.6961472
H	6.0903743	2.7206630	-3.0664666
H	5.3748589	3.4697372	-0.8154135
H	8.0632665	6.7149317	1.4787080
H	9.2333496	8.8918579	1.8539215
H	8.0378618	11.0539472	1.4255206
H	5.6571775	11.0320605	0.6329556
H	4.4723109	8.8331941	0.2898029

S2

75

SCF Energy = -4548.280053094

C	0.3437317	4.5145154	-3.0225382
C	-0.0098208	3.9110200	-1.7993152
C	-0.9943911	2.8958428	-1.7911874

C	-1.5833420	2.4712422	-2.9891068
C	-1.1961425	3.0538381	-4.2102830
C	-0.2336054	4.0758342	-4.2231971
C	0.6310963	4.3119660	-0.5223690
C	1.6190092	3.6628360	0.1983447
C	2.5113083	2.6919113	-0.5000559
C	2.0512541	1.6737399	-1.3661774
C	2.9555757	0.8371920	-2.0360492
C	4.3410414	0.9877549	-1.8566436
C	4.8137486	1.9813227	-0.9827169
C	3.9124736	2.8176125	-0.3114831
Br	-0.7326088	5.5446429	0.5320736
C	0.7923698	1.5239067	2.0748280
C	2.0256481	0.6766472	2.2599400
C	-0.3442468	1.0328361	1.5366029
C	0.8829388	2.9682544	2.5126491
C	1.8965420	3.8289779	1.7046818
O	1.9546365	5.1486420	2.2195178
H	2.9102440	3.4205785	1.8791530
H	-0.1133843	3.4478134	2.4300811
H	1.1968788	3.0341466	3.5776161
H	-1.2391631	1.6655266	1.4237243
H	-0.4204864	-0.0152317	1.2063030
H	2.3604698	0.6931382	3.3196670
H	2.8726889	1.0590276	1.6517184
H	1.8497408	-0.3751794	1.9641050
H	1.0669060	5.5495881	2.0938655
H	0.9752211	1.5253781	-1.5063546
H	2.5677527	0.0522597	-2.7033106
H	5.0463958	0.3325015	-2.3895788
H	5.8935047	2.1270991	-0.8310359
H	4.3036249	3.6161989	0.3328049
H	-1.2783421	2.4377190	-0.8324443
H	-2.3446077	1.6765635	-2.9726180
H	-1.6538168	2.7133651	-5.1517435
H	0.0766182	4.5400885	-5.1709959
H	1.0849565	5.3248199	-3.0141923
Pd	1.6149445	6.1964496	-0.5617893
P	3.4958004	6.8363886	-1.6308356
C	4.9735382	6.1544688	-0.7641524
C	6.0976681	5.6415328	-1.4427158
H	6.1284938	5.6573323	-2.5423708
C	7.1612964	5.0782138	-0.7189109
H	8.0302963	4.6683627	-1.2561915
C	7.1145022	5.0314020	0.6847354
H	7.9463395	4.5827990	1.2489608

C	5.9979205	5.5481749	1.3656759
H	5.9476404	5.5011543	2.4640050
C	4.9275927	6.1002821	0.6458470
H	4.0199289	6.4393789	1.1709682
C	3.9416907	8.5904466	-1.9802476
C	5.2698634	9.0128537	-2.1927931
H	6.0950772	8.2887341	-2.1192305
C	5.5394853	10.3576778	-2.4893675
H	6.5786189	10.6844545	-2.6482356
C	4.4875171	11.2859052	-2.5824464
H	4.7030283	12.3401495	-2.8141337
C	3.1628991	10.8689653	-2.3689910
H	2.3376921	11.5945488	-2.4322311
C	2.8912744	9.5269261	-2.0587808
H	1.8610060	9.1856864	-1.8633149
C	3.5820764	6.0515141	-3.2949308
C	3.6197998	4.6398794	-3.3664348
H	3.6889177	4.0452602	-2.4451399
C	3.5496164	3.9918187	-4.6057374
H	3.5761265	2.8925203	-4.6377034
C	3.4242396	4.7413049	-5.7892540
H	3.3583337	4.2318701	-6.7626534
C	3.3811660	6.1439668	-5.7233395
H	3.2855885	6.7372648	-6.6457393
C	3.4638377	6.8000941	-4.4830748
H	3.4315279	7.8988647	-4.4380171

S3

75

SCF Energy = -4548.278838502

C	0.4844363	3.8250301	-2.9037465
C	-0.1523029	3.9341996	-1.6403151
C	-1.5598315	3.8343659	-1.5792302
C	-2.3080579	3.6211381	-2.7456489
C	-1.6682172	3.5083765	-3.9914648
C	-0.2683190	3.6118833	-4.0641451
C	0.7002099	4.1317765	-0.4450730
C	1.7355919	3.3327791	-0.0218829
C	2.0883973	2.1543209	-0.8672643
C	1.1639281	1.1183282	-1.1233586
C	1.5087307	0.0473701	-1.9592615
C	2.7803253	-0.0040313	-2.5560613
C	3.7055612	1.0240546	-2.3089276
C	3.3648127	2.0942413	-1.4699214
Br	-0.3668868	5.4110202	1.0568282
C	0.9896311	2.5209595	2.9622059

C	-0.2111826	1.8916029	2.3036645
C	0.8898321	3.2417889	4.1006417
C	2.3248201	2.3657003	2.2666596
C	2.6149544	3.4898698	1.2211763
O	2.6313740	4.7575289	1.8341674
H	3.6560982	3.3217816	0.8698606
H	3.1459903	2.4151509	3.0090262
H	2.3927763	1.3831576	1.7545165
H	1.7769764	3.6954998	4.5697048
H	-0.0803700	3.3977665	4.5983976
H	-0.0481873	0.8052806	2.1371584
H	-0.3920377	2.3446301	1.3064477
H	-1.1287474	2.0231405	2.9083453
H	1.7129353	4.9630350	2.1254941
H	0.1640222	1.1669011	-0.6695247
H	0.7764609	-0.7518275	-2.1502843
H	3.0470670	-0.8421120	-3.2176464
H	4.6974009	1.0058094	-2.7849741
H	4.0766940	2.9199725	-1.3184825
H	-2.0609609	3.9339004	-0.6064968
H	-3.4039829	3.5441286	-2.6798731
H	-2.2601279	3.3441760	-4.9046126
H	0.2441574	3.5276271	-5.0344455
H	1.5795231	3.8921616	-2.9547303
Pd	1.5467011	5.9768582	-0.6588055
P	3.2443664	7.2168649	-1.5320372
C	3.0209825	8.5144853	-2.8152381
C	3.9522622	8.7321485	-3.8527832
H	4.8433998	8.0909747	-3.9317494
C	3.7361438	9.7564748	-4.7878173
H	4.4636909	9.9201720	-5.5975551
C	2.5940198	10.5701114	-4.6918595
H	2.4258768	11.3710584	-5.4278718
C	1.6623832	10.3539314	-3.6623313
H	0.7623336	10.9832228	-3.5906139
C	1.8709625	9.3254161	-2.7306524
H	1.1378078	9.1309190	-1.9313536
C	4.4447003	7.9456655	-0.3418191
C	4.5237289	7.3477737	0.9352816
H	3.8541938	6.5076660	1.1901166
C	5.4517672	7.8275547	1.8729721
H	5.5124523	7.3547805	2.8651336
C	6.2859449	8.9129297	1.5540642
H	7.0040882	9.2943566	2.2960824
C	6.1946383	9.5180339	0.2891029
H	6.8399032	10.3739359	0.0383552

C	5.2799606	9.0350575	-0.6604384
H	5.2113245	9.5117861	-1.6494508
C	4.2553533	5.9383084	-2.4089861
C	3.7324592	5.3671978	-3.5919841
H	2.7861316	5.7484868	-4.0061964
C	4.4114780	4.3250784	-4.2373306
H	3.9936829	3.8879349	-5.1567719
C	5.6192736	3.8343964	-3.7086662
H	6.1517890	3.0158637	-4.2159012
C	6.1408394	4.3944866	-2.5317027
H	7.0861146	4.0169331	-2.1126872
C	5.4654696	5.4438486	-1.8836080
H	5.8807784	5.8814894	-0.9640550

S4

75

SCF Energy = -4548.276842071

C	0.3639818	3.9519859	-2.8787243
C	-0.1213569	4.0365486	-1.5473428
C	-1.5173935	4.0434456	-1.3315125
C	-2.4025196	3.9603342	-2.4151131
C	-1.9131672	3.8730248	-3.7298383
C	-0.5260977	3.8688584	-3.9558800
C	0.8661009	4.1042686	-0.4482598
C	1.8648577	3.2112802	-0.1513259
C	2.0239794	2.0398159	-1.0625033
C	0.9641869	1.1394806	-1.3101312
C	1.1282413	0.0741429	-2.2054262
C	2.3513478	-0.1067671	-2.8745260
C	3.4086155	0.7882538	-2.6405890
C	3.2485750	1.8523436	-1.7416733
Br	0.0854266	5.4533398	1.2013438
C	1.2249764	2.2884419	2.7679795
C	1.2685304	3.1440581	4.0093043
C	0.0856288	1.7152394	2.3270390
C	2.5322040	2.1052201	2.0258295
C	2.8622778	3.2428647	1.0078760
O	3.0680452	4.4863458	1.6481345
H	3.8469209	2.9778772	0.5646342
H	3.3805601	2.0675987	2.7411077
H	2.5255024	1.1475334	1.4667572
H	0.0801410	1.0667927	1.4377971
H	-0.8746833	1.8745958	2.8422594
H	1.7496484	4.1219600	3.8062172
H	1.8902061	2.6558403	4.7919806
H	0.2595390	3.3226655	4.4278763

H	2.1887113	4.9042559	1.8038557
H	0.0012811	1.2948668	-0.8035887
H	0.2922613	-0.6186650	-2.3857469
H	2.4771975	-0.9405993	-3.5816829
H	4.3644992	0.6705630	-3.1727788
H	4.0660299	2.5752362	-1.5996258
H	-1.8974422	4.1192187	-0.3034560
H	-3.4874817	3.9645897	-2.2303266
H	-2.6125902	3.8110182	-4.5772708
H	-0.1315911	3.8010124	-4.9810372
H	1.4493542	3.9278047	-3.0475691
Pd	1.8168938	5.8872053	-0.7325369
P	3.5549157	7.0041918	-1.6935570
C	4.8730281	7.6422724	-0.5791868
C	5.0195314	7.0043156	0.6725769
H	4.3393885	6.1810482	0.9530513
C	6.0315715	7.4195123	1.5520871
H	6.1443154	6.9151025	2.5238852
C	6.8845485	8.4805695	1.2020886
H	7.6691536	8.8117240	1.8995568
C	6.7276547	9.1251183	-0.0364571
H	7.3879894	9.9618841	-0.3113394
C	5.7279756	8.7063074	-0.9293189
H	5.6088074	9.2136500	-1.8980225
C	4.4124759	5.6556606	-2.6275429
C	3.7769059	5.1300864	-3.7760531
H	2.8386446	5.5833555	-4.1321646
C	4.3360190	4.0439750	-4.4623784
H	3.8308313	3.6427611	-5.3538667
C	5.5345330	3.4633615	-4.0093990
H	5.9727004	2.6099757	-4.5484425
C	6.1668273	3.9771772	-2.8662386
H	7.1053954	3.5287923	-2.5060831
C	5.6121354	5.0703613	-2.1773781
H	6.1144385	5.4714178	-1.2850524
C	3.3481642	8.3165559	-2.9637695
C	4.2347977	8.4729383	-4.0502767
H	5.0764866	7.7746370	-4.1744443
C	4.0369654	9.5101038	-4.9749877
H	4.7292797	9.6261814	-5.8229311
C	2.9578217	10.3973976	-4.8199940
H	2.8036846	11.2083107	-5.5481198
C	2.0708756	10.2428461	-3.7411559
H	1.2198039	10.9305054	-3.6227387
C	2.2609238	9.2020837	-2.8190483
H	1.5611024	9.0566297	-1.9804032

Optimized Geometries(BXnb)

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R1
75
SCF Energy = -4548.320737654
C      1.5447813   -0.3125753   -2.3753259
C      1.3985209    0.3697932   -1.1423771
C      0.9723511    1.7196579   -1.1519853
C      0.7044316    2.3672917   -2.3636460
C      0.8630063    1.6830655   -3.5820386
C      1.2903979    0.3446150   -3.5841706
C      1.6931816   -0.3485422    0.1046717
C      2.8744852   -0.9185349    0.4442537
C      4.0766693   -0.6119260   -0.3977299
C      4.9273353   -1.6483819   -0.8464536
C      6.0496293   -1.3542034   -1.6362808
C      6.3473678   -0.0266157   -1.9845086
C      5.5189631    1.0111721   -1.5246050
C      4.3970457    0.7220162   -0.7364293
Br     0.2888609    1.7485225    2.4778255
C      0.6980376   -1.9246172    2.4859155
C     -0.1913528   -1.8688303    3.7142710
C      0.1675420   -2.5178554    1.2907925
C      2.1699540   -1.7525734    2.7865844
C      3.1421909   -1.8667642    1.6159799
O      3.2784214   -3.2286706    1.1692924
H      4.1532695   -1.6175707    1.9977002
H      2.3002687   -0.7660616    3.2809433
H      2.4771037   -2.5221366    3.5311696
H      0.8164492   -2.8877600    0.4809488
H     -0.8396473   -2.9680945    1.3141424
H      0.0046891   -0.9507959    4.3026752
H      0.0175559   -2.7444823    4.3697747
H     -1.2671322   -1.8939527    3.4511516
H      2.3837165   -3.5335081    0.9262409
H      4.6893881   -2.6843297   -0.5674294
H      6.6963974   -2.1741251   -1.9852933
H      7.2268775    0.2001340   -2.6062944
H      5.7511771    2.0572281   -1.7765749
H      3.7581611    1.5364774   -0.3670858
H      0.8640398    2.2384020   -0.1878147
H      0.3669717    3.4144534   -2.3566768
H      0.6455143    2.1927094   -4.5328683
H      1.4095773   -0.1967130   -4.5338537

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H	1.8806748	-1.3586226	-2.3666090
Pd	-0.0041368	-0.4098009	1.1706244
P	-1.8359791	0.0962971	-0.3732356
C	-2.7253619	1.6900229	-0.5768114
C	-2.1338679	2.8703515	-0.0866949
H	-1.1657104	2.8166349	0.4336529
C	-2.8113044	4.0951385	-0.2103424
H	-2.3484885	5.0130771	0.1823606
C	-4.0757257	4.1455720	-0.8177821
H	-4.6035647	5.1067522	-0.9140543
C	-4.6787661	2.9641162	-1.2870917
H	-5.6789333	2.9984394	-1.7454580
C	-4.0106152	1.7381749	-1.1609092
H	-4.4898292	0.8102768	-1.5095584
C	-1.7535174	-0.6413111	-2.0457440
C	-1.2067892	-1.9404906	-2.1582915
H	-0.8932150	-2.4735514	-1.2486592
C	-1.0445449	-2.5377560	-3.4150719
H	-0.6259821	-3.5530301	-3.4872364
C	-1.3939978	-1.8324397	-4.5798937
H	-1.2566795	-2.2959460	-5.5684973
C	-1.9067297	-0.5300993	-4.4762523
H	-2.1651919	0.0348538	-5.3846881
C	-2.0890431	0.0645177	-3.2174155
H	-2.4788888	1.0893579	-3.1474140
C	-3.0851600	-0.9006314	0.5489470
C	-3.3189097	-0.4993055	1.8865305
H	-2.8278365	0.4075510	2.2782849
C	-4.1602713	-1.2564154	2.7135003
H	-4.3349544	-0.9356945	3.7516643
C	-4.7729307	-2.4224274	2.2197037
H	-5.4287813	-3.0198545	2.8707317
C	-4.5478261	-2.8192250	0.8913904
H	-5.0330069	-3.7255062	0.4975377
C	-3.7085237	-2.0627407	0.0552801
H	-3.5389030	-2.3771488	-0.9850391

R2

75

SCF Energy = -4548.309398392

C	1.7333764	1.9158247	-2.1015977
C	0.9644016	1.8557860	-0.9060919
C	-0.0860597	2.8032859	-0.7728300
C	-0.4171911	3.6927055	-1.8026910
C	0.3190044	3.6942637	-2.9978555
C	1.4092167	2.8153284	-3.1240993

C	1.2006340	0.8759860	0.1708778
C	2.2282741	0.0109522	0.3840676
C	3.1374494	-0.3963544	-0.7278663
C	2.6348622	-1.2593068	-1.7279277
C	3.4657204	-1.7106288	-2.7610839
C	4.8134866	-1.3112615	-2.8097173
C	5.3229446	-0.4570955	-1.8176032
C	4.4933223	-0.0018805	-0.7780602
Br	0.6587303	2.0685956	3.3259521
C	1.9459258	-3.1202428	1.0654886
C	3.3444110	-3.5987478	0.7535703
C	0.8611557	-3.7459326	0.5617308
C	1.7786591	-1.9650905	2.0261545
C	2.5305525	-0.6423441	1.7493462
O	3.9305850	-0.7541947	1.9708755
H	2.1795186	0.0748560	2.5178266
H	0.7012052	-1.7132397	2.1060045
H	2.1140623	-2.2831140	3.0395045
H	-0.1541606	-3.4165927	0.8295861
H	0.9534828	-4.6167722	-0.1069288
H	3.9298846	-3.7554812	1.6839243
H	3.9000804	-2.8630548	0.1317391
H	3.3315872	-4.5478419	0.1833714
H	4.2976428	-1.3467818	1.2864650
H	1.5850086	-1.5735575	-1.6752984
H	3.0555916	-2.3806366	-3.5317737
H	5.4670224	-1.6652130	-3.6215677
H	6.3752654	-0.1361846	-1.8540425
H	4.8809203	0.6773624	-0.0064963
H	-0.6486165	2.8302195	0.1717020
H	-1.2567540	4.3897248	-1.6614653
H	0.0603899	4.3851319	-3.8144499
H	2.0163665	2.8178190	-4.0424732
H	2.5730951	1.2312106	-2.2496139
Pd	-0.2966049	0.8048829	1.5079180
P	-1.6858375	-0.1849375	-0.0337970
C	-2.6138798	-1.5681223	0.7520725
C	-3.0216911	0.9909385	-0.5173011
C	-1.1148392	-0.8766844	-1.6353637
C	-3.6919795	-2.2010341	0.0980260
C	-4.3755552	-3.2502104	0.7279614
C	-3.9957390	-3.6689246	2.0165520
C	-2.9328949	-3.0334063	2.6769441
C	-2.2436501	-1.9847747	2.0459732
H	-3.9958961	-1.8717850	-0.9068213
H	-5.2132765	-3.7437080	0.2124524

H	-4.5356494	-4.4924612	2.5078326
H	-2.6346406	-3.3528635	3.6864789
H	-1.4069232	-1.4789982	2.5564238
C	-3.7231593	0.8905333	-1.7357472
C	-4.7434756	1.8066539	-2.0374479
C	-5.0746739	2.8226167	-1.1259877
C	-4.3836426	2.9212363	0.0939908
C	-3.3603593	2.0116767	0.3956467
H	-3.4604229	0.1063133	-2.4606475
H	-5.2801662	1.7274185	-2.9950126
H	-5.8709181	3.5425317	-1.3684206
H	-4.6351019	3.7164577	0.8116008
H	-2.8010710	2.1017035	1.3421250
C	-0.9490399	-2.2666152	-1.8063878
C	-0.4359205	-2.7762165	-3.0094547
C	-0.0822436	-1.9037516	-4.0515080
C	-0.2561107	-0.5192685	-3.8900178
C	-0.7719075	-0.0045137	-2.6924640
H	-1.2267459	-2.9552490	-0.9992807
H	-0.3081267	-3.8626201	-3.1266018
H	0.3254751	-2.3030573	-4.9924078
H	0.0176645	0.1751759	-4.6976812
H	-0.9165517	1.0785423	-2.5859975

R3

75

SCF Energy = -4548.318865396

C	1.5445026	2.1603760	-2.0883332
C	1.4017818	0.8117257	-1.6787224
C	1.2740795	-0.1868111	-2.6730932
C	1.2962916	0.1503693	-4.0320920
C	1.4501496	1.4896050	-4.4267090
C	1.5779804	2.4916262	-3.4490168
C	1.3859127	0.4912912	-0.2406307
C	2.2448330	-0.2759971	0.4739087
C	3.3205636	-1.0421012	-0.2153971
C	3.4790567	-2.4236730	0.0589354
C	4.4760613	-3.1755229	-0.5846690
C	5.3320765	-2.5628774	-1.5131937
C	5.1893867	-1.1905896	-1.7857762
C	4.1996159	-0.4371021	-1.1413587
Br	1.0706566	3.2582565	1.5791502
C	0.0572497	-1.0457796	3.4177625
C	-0.8799706	-2.1717324	3.7811883
C	-0.1379991	0.2091518	3.8791209
C	1.2032032	-1.4764531	2.5246614

C	2.1867284	-0.3923548	2.0061783
O	3.4887632	-0.5410111	2.5587748
H	1.8459919	0.6007263	2.3561770
H	1.8112790	-2.2164423	3.0929151
H	0.7614896	-2.0456114	1.6817426
H	0.5227671	1.0536192	3.6363413
H	-0.9840325	0.4277762	4.5503068
H	-1.3301795	-2.6189579	2.8695979
H	-1.6990123	-1.8356540	4.4462693
H	-0.3321519	-2.9929275	4.2926469
H	3.9381300	-1.2540835	2.0616630
H	2.7959719	-2.9202010	0.7651565
H	4.5789345	-4.2485805	-0.3611455
H	6.1130762	-3.1505318	-2.0187369
H	5.8641259	-0.6993205	-2.5033501
H	4.1005372	0.6380224	-1.3448930
H	1.1652122	-1.2390056	-2.3780623
H	1.1870011	-0.6404305	-4.7891293
H	1.4631129	1.7523401	-5.4952947
H	1.6989065	3.5438308	-3.7486457
H	1.6253057	2.9365269	-1.3117595
Pd	-0.1409254	1.3481366	0.6926974
P	-1.6342613	-0.1181509	-0.1806034
C	-1.8793030	0.0870381	-1.9840900
C	-1.7294971	1.3852225	-2.5159325
H	-1.4576001	2.2161754	-1.8458714
C	-1.8869039	1.6001275	-3.8903542
H	-1.7520314	2.6107934	-4.3021440
C	-2.1877356	0.5227268	-4.7418820
H	-2.2959328	0.6914014	-5.8239700
C	-2.3387416	-0.7696351	-4.2145777
H	-2.5716560	-1.6145390	-4.8802178
C	-2.1861765	-0.9911585	-2.8365567
H	-2.2949757	-2.0048168	-2.4239953
C	-3.2451040	0.3326385	0.5718166
C	-3.2832466	0.4999206	1.9744251
H	-2.3635755	0.3527250	2.5639567
C	-4.4857017	0.8533720	2.6031678
H	-4.5113028	0.9845954	3.6953530
C	-5.6491194	1.0507340	1.8391445
H	-6.5902860	1.3357001	2.3332535
C	-5.6095146	0.8919241	0.4434126
H	-6.5190222	1.0501964	-0.1557049
C	-4.4110033	0.5334322	-0.1939667
H	-4.3766598	0.4104048	-1.2865092
C	-1.5300488	-1.9382118	0.0343144

C	-2.6195345	-2.6901978	0.5182623
H	-3.5550450	-2.1830906	0.7953875
C	-2.5084586	-4.0842004	0.6524821
H	-3.3619824	-4.6627105	1.0368183
C	-1.3159747	-4.7369978	0.2994059
H	-1.2327660	-5.8290414	0.4060261
C	-0.2289088	-3.9910487	-0.1877323
H	0.7123638	-4.4906629	-0.4618784
C	-0.3316719	-2.5984988	-0.3139038
H	0.5297142	-2.0144496	-0.6647833

R4

75

SCF Energy = -4548.324435477

C	5.5763538	0.7332095	0.3098261
C	4.5793736	-0.1898601	-0.0949790
C	4.8566405	-1.0386169	-1.1937247
C	6.0787867	-0.9602413	-1.8746467
C	7.0575901	-0.0379028	-1.4667032
C	6.7999806	0.8050126	-0.3726295
C	3.2573403	-0.2388009	0.5797835
Pd	0.2151601	-0.3719367	0.4807162
P	-2.1139392	-0.3153619	-0.1020525
C	2.1189989	-0.3357046	-0.1322580
Br	0.3805043	2.1316975	0.8675160
C	1.7771750	-0.1994107	-1.5478409
C	2.0400719	1.0067084	-2.2526224
C	1.5321945	1.1955393	-3.5412535
C	0.7277231	0.2077374	-4.1475682
C	0.4569322	-0.9893194	-3.4681751
C	0.9897960	-1.2008339	-2.1866747
C	3.1506091	-0.2489829	2.1062645
O	4.3956017	-0.1995861	2.7787086
C	2.3471081	-1.5172379	2.5295593
C	0.8498259	-1.4696857	2.3178711
C	0.2074213	-2.3502240	1.4133086
C	0.0632182	-0.7920190	3.4196452
H	2.5868463	0.6527672	2.4308238
H	2.5339695	-1.6408180	3.6167510
H	2.7882072	-2.3917787	2.0091913
H	0.8120963	-3.0792010	0.8494313
H	-0.8417082	-2.6302717	1.5988914
H	0.1987354	-1.3520959	4.3718564
H	-1.0181759	-0.7506058	3.1928101
H	0.4206448	0.2439960	3.5849140
H	4.9942586	-0.8322663	2.3350123

H	4.0958995	-1.7686174	-1.5063885
H	6.2716746	-1.6300828	-2.7266655
H	8.0192797	0.0219988	-1.9985617
H	7.5577510	1.5353295	-0.0494925
H	5.3767711	1.3995845	1.1594133
H	0.7994049	-2.1466600	-1.6604393
H	-0.1774747	-1.7626763	-3.9262538
H	0.3081852	0.3800199	-5.1501786
H	1.7428753	2.1342879	-4.0758314
H	2.6163195	1.7944053	-1.7482050
C	-2.6395756	1.2448850	-0.9042209
C	-3.3164431	-0.5733645	1.2510133
C	-2.5212049	-1.5714379	-1.3910930
C	-3.2430579	-1.2283149	-2.5528844
C	-3.4517393	-2.1798403	-3.5642721
C	-2.9490579	-3.4835931	-3.4265598
C	-2.2366412	-3.8351936	-2.2667112
C	-2.0180300	-2.8841183	-1.2598069
H	-3.6305904	-0.2068870	-2.6728161
H	-4.0100051	-1.8959130	-4.4693179
H	-3.1095985	-4.2259441	-4.2230025
H	-1.8372582	-4.8541206	-2.1502755
H	-1.4347780	-3.1556869	-0.3702682
C	-3.9082897	1.8182977	-0.6976149
C	-4.2682548	2.9867627	-1.3899067
C	-3.3692319	3.5754237	-2.2943847
C	-2.1038611	2.9992570	-2.5028670
C	-1.7322289	1.8444092	-1.8025931
H	-4.6154045	1.3522619	0.0046998
H	-5.2580861	3.4375976	-1.2213985
H	-3.6534405	4.4915105	-2.8343859
H	-1.3904454	3.4616068	-3.2012570
H	-0.7342457	1.4081016	-1.9484480
C	-4.2255706	-1.6477224	1.2896601
C	-5.0654650	-1.8135162	2.4045436
C	-5.0077927	-0.9063447	3.4745534
C	-4.1028693	0.1707970	3.4343859
C	-3.2516294	0.3349524	2.3334443
H	-4.2787864	-2.3510882	0.4451793
H	-5.7738246	-2.6555117	2.4324286
H	-5.6688805	-1.0378427	4.3444678
H	-4.0542454	0.8834509	4.2715430
H	-2.5270642	1.1656034	2.3009965

S1
75

SCF Energy = -4548.326624207

C	0.8898678	0.9904195	-2.5390340
C	1.2526621	1.4050645	-1.2351622
C	1.4869964	2.7878131	-1.0082767
C	1.3397167	3.7178565	-2.0440572
C	0.9492497	3.2942422	-3.3282886
C	0.7353417	1.9281407	-3.5702981
C	1.3526856	0.4741415	-0.0941360
C	2.3128395	-0.4234116	0.2194454
C	3.4362594	-0.6319983	-0.7468779
C	3.2254067	-1.2418005	-2.0008204
C	4.2980142	-1.4513246	-2.8821485
C	5.5958392	-1.0578229	-2.5190632
C	5.8169451	-0.4655295	-1.2630920
C	4.7484578	-0.2563200	-0.3793281
Br	1.2159312	2.3573957	2.7821161
C	0.7779592	-3.0063356	1.7171385
C	-0.4286738	-3.5556508	2.4357234
C	1.3378814	-3.6560871	0.6717176
C	1.2933831	-1.6974616	2.2602688
C	2.5366724	-1.1026341	1.5886577
O	3.2416933	-0.2213079	2.4517713
H	3.2481500	-1.9343112	1.4081045
H	0.4607382	-0.9451571	2.2450807
H	1.5413922	-1.8230591	3.3370597
H	2.2098607	-3.2634093	0.1272864
H	0.9277102	-4.6173729	0.3230824
H	-1.2720143	-2.8356740	2.3910878
H	-0.2093522	-3.7096464	3.5142277
H	-0.7692865	-4.5174208	2.0067391
H	2.6685563	0.5714325	2.6058391
H	2.2126076	-1.5692931	-2.2730766
H	4.1169346	-1.9281659	-3.8577897
H	6.4365493	-1.2171009	-3.2114266
H	6.8329782	-0.1597609	-0.9694317
H	4.9049725	0.1960733	0.6110576
H	1.7640993	3.1154126	0.0048962
H	1.5258031	4.7841622	-1.8453981
H	0.8201146	4.0276614	-4.1386772
H	0.4438501	1.5813355	-4.5730953
H	0.7247055	-0.0721252	-2.7424007
Pd	-0.0744337	1.0164222	1.1945064
P	-1.7557550	0.0976030	-0.0167299
C	-2.8566793	1.4730375	-0.5296289
C	-2.2562477	2.6163727	-1.1033637
H	-1.1620224	2.6743256	-1.2016278

C	-3.0596043	3.6768151	-1.5447760
H	-2.5861812	4.5628872	-1.9931295
C	-4.4570788	3.6112338	-1.4043331
H	-5.0845202	4.4495117	-1.7431994
C	-5.0531654	2.4788689	-0.8243438
H	-6.1464520	2.4282285	-0.7087743
C	-4.2571025	1.4073256	-0.3883379
H	-4.7225135	0.5190421	0.0641297
C	-1.4917895	-0.8597498	-1.5496255
C	-0.6164962	-1.9632900	-1.4926421
H	-0.1396034	-2.2503146	-0.5435631
C	-0.3278358	-2.6869735	-2.6579510
H	0.3591093	-3.5450892	-2.6039565
C	-0.8990312	-2.3068681	-3.8857772
H	-0.6591984	-2.8661288	-4.8027483
C	-1.7765591	-1.2107484	-3.9402687
H	-2.2273756	-0.9112811	-4.8983710
C	-2.0777574	-0.4871371	-2.7752508
H	-2.7519358	0.3797187	-2.8224694
C	-2.8002290	-0.9851954	1.0316875
C	-2.9346409	-0.6485709	2.3965115
H	-2.4171620	0.2394218	2.7960465
C	-3.7052496	-1.4522875	3.2478275
H	-3.8010747	-1.1865293	4.3110459
C	-4.3372160	-2.6037801	2.7455163
H	-4.9309095	-3.2422681	3.4167949
C	-4.2032480	-2.9431307	1.3892811
H	-4.6934401	-3.8461606	0.9954107
C	-3.4402440	-2.1357194	0.5300069
H	-3.3297222	-2.4047028	-0.5305628

S2

75

SCF Energy = -4548.323676785

C	2.0413866	2.0597133	-1.7571702
C	1.4483376	0.8102762	-1.4525116
C	0.8465255	0.0732792	-2.4985518
C	0.8599744	0.5564043	-3.8130501
C	1.4597219	1.7917448	-4.1052670
C	2.0494719	2.5413902	-3.0720798
C	1.4866465	0.3432588	-0.0523746
C	2.4558601	-0.4037093	0.5301351
C	3.5255869	-0.9828450	-0.3447661
C	3.2202572	-1.8899118	-1.3819265
C	4.2367634	-2.4403042	-2.1775848
C	5.5778467	-2.0953202	-1.9457932

C	5.8942051	-1.2045989	-0.9053709
C	4.8805890	-0.6543353	-0.1075439
Br	1.4987641	3.0082940	2.0106178
C	0.6682294	-1.9840997	2.7027307
C	1.3533791	-3.2579167	2.2797117
C	-0.6680420	-1.9140048	2.8730166
C	1.5403029	-0.7805642	2.9757878
C	2.7394278	-0.5784734	2.0354221
O	3.5668609	0.4841035	2.4916693
H	3.3806923	-1.4806079	2.1130570
H	0.9156232	0.1393445	2.9982565
H	1.9903667	-0.8723894	3.9900746
H	-1.1434767	-0.9716922	3.1867540
H	-1.3193217	-2.7876643	2.7114128
H	2.1355134	-3.5550424	3.0116803
H	1.8775972	-3.1297264	1.3070416
H	0.6360984	-4.0943581	2.1769306
H	3.0360537	1.3163036	2.4056112
H	2.1737204	-2.1733084	-1.5601333
H	3.9776162	-3.1452318	-2.9824489
H	6.3758095	-2.5226477	-2.5719860
H	6.9433744	-0.9305466	-0.7148461
H	5.1133216	0.0416011	0.7117529
H	0.3587945	-0.8858274	-2.2783928
H	0.3863396	-0.0320454	-4.6125499
H	1.4617795	2.1738922	-5.1372116
H	2.5204328	3.5113994	-3.2927048
H	2.4834847	2.6442969	-0.9366249
Pd	0.0781662	1.2882222	0.9913823
P	-1.6752994	0.2717403	-0.0201003
C	-1.9527968	1.0198754	-1.6777205
C	-1.4422823	2.3171069	-1.8997731
H	-0.8733968	2.8179100	-1.0987997
C	-1.6078583	2.9339452	-3.1463450
H	-1.1909433	3.9374204	-3.3152454
C	-2.2756877	2.2587349	-4.1817444
H	-2.3920819	2.7372843	-5.1658461
C	-2.7799682	0.9659928	-3.9652438
H	-3.2951935	0.4311516	-4.7774964
C	-2.6209390	0.3447732	-2.7168344
H	-2.9984067	-0.6759003	-2.5605576
C	-1.8617935	-1.5299125	-0.2731203
C	-3.1280947	-2.1311374	-0.4353901
H	-4.0413818	-1.5219963	-0.3608065
C	-3.2221290	-3.5104559	-0.6801349
H	-4.2115603	-3.9766899	-0.8012511

C	-2.0575824	-4.2918483	-0.7731460
H	-2.1349344	-5.3721469	-0.9683891
C	-0.7963677	-3.6950035	-0.6077728
H	0.1179645	-4.3041130	-0.6649737
C	-0.6979383	-2.3209472	-0.3460782
H	0.2803167	-1.8515670	-0.1702638
C	-3.1464978	0.7863966	0.9560507
C	-3.6157423	-0.0186029	2.0176420
H	-3.1611285	-1.0015721	2.2017450
C	-4.6671746	0.4302823	2.8294710
H	-5.0296805	-0.2069328	3.6501138
C	-5.2523789	1.6870985	2.5993341
H	-6.0744203	2.0385857	3.2407445
C	-4.7856429	2.4924744	1.5474224
H	-5.2418269	3.4759882	1.3595105
C	-3.7383047	2.0474000	0.7270678
H	-3.3831649	2.6785901	-0.1006870

S3

75

SCF Energy = -4548.302784434

C	1.5486570	-0.6713482	-2.0521954
C	1.3211888	-1.3584914	-0.8344892
C	1.0363107	-2.7453075	-0.8648773
C	1.0105080	-3.4376311	-2.0810241
C	1.2636819	-2.7523821	-3.2839053
C	1.5306334	-1.3733809	-3.2636327
C	1.4172816	-0.6246890	0.4216175
C	2.4343250	0.1516690	0.8653049
C	3.7424426	0.1745275	0.1564933
C	4.4271992	-1.0117949	-0.1845374
C	5.6511649	-0.9591140	-0.8665965
C	6.2070648	0.2817672	-1.2209320
C	5.5271651	1.4677433	-0.8939014
C	4.3045303	1.4201154	-0.2085976
Br	0.7934913	2.8221558	-0.4232654
C	1.6981970	-1.2387661	3.3870161
C	2.3362436	-2.5368038	2.9799379
C	0.3727896	-1.1686597	3.7616251
C	2.5856310	-0.0195247	3.3800815
C	2.3304098	0.9367688	2.1684740
O	1.0833697	1.5542683	2.3637617
H	3.1552215	1.6856347	2.1872932
H	2.4168346	0.5896274	4.2909364
H	3.6496273	-0.3267181	3.3578010
H	-0.0257281	-0.2480047	4.2189818

H	-0.2151830	-2.0948352	3.8841430
H	2.8272082	-2.4249385	1.9911592
H	1.6095823	-3.3699954	2.9289933
H	3.1375971	-2.8025348	3.7029167
H	0.8956586	2.0638127	1.4906604
H	3.9860287	-1.9838894	0.0820818
H	6.1737731	-1.8932385	-1.1235314
H	7.1669471	0.3240920	-1.7580564
H	5.9454360	2.4425239	-1.1883042
H	3.7308592	2.3388566	-0.0088576
H	0.8548303	-3.2702130	0.0859265
H	0.7967756	-4.5172774	-2.0949248
H	1.2402336	-3.2946855	-4.2411585
H	1.7082985	-0.8334858	-4.2051986
H	1.7282390	0.4141147	-2.0095841
Pd	-0.1826198	-0.6561195	1.6150316
P	-1.7313559	-0.1668898	0.0149495
C	-1.6178302	-0.3088271	-1.8024497
C	-1.1779829	0.8185045	-2.5324579
H	-0.8511931	1.7272785	-1.9940879
C	-1.1121308	0.7512824	-3.9310318
H	-0.7706420	1.6327749	-4.4943418
C	-1.4588561	-0.4316677	-4.6038627
H	-1.4010189	-0.4805681	-5.7020731
C	-1.8748837	-1.5571030	-3.8730824
H	-2.1411143	-2.4888905	-4.3941399
C	-1.9606761	-1.4988002	-2.4748091
H	-2.3065532	-2.3775439	-1.9134922
C	-2.5171943	1.4537027	0.3124597
C	-2.1382904	2.1950412	1.4484129
H	-1.3317527	1.8204179	2.0972532
C	-2.7613134	3.4203015	1.7227528
H	-2.4495198	4.0033332	2.6016625
C	-3.7524856	3.9146223	0.8591740
H	-4.2294056	4.8844719	1.0671194
C	-4.1254055	3.1806489	-0.2796535
H	-4.8945704	3.5719467	-0.9625522
C	-3.5110748	1.9497856	-0.5564404
H	-3.7943515	1.3799208	-1.4536765
C	-3.0007764	-1.4063178	0.5267746
C	-4.3124328	-1.0426560	0.8939114
H	-4.6193351	0.0122847	0.8508186
C	-5.2211613	-2.0253673	1.3197411
H	-6.2418925	-1.7320016	1.6082961
C	-4.8330479	-3.3735930	1.3793081
H	-5.5491013	-4.1394539	1.7136822

C	-3.5241984	-3.7418705	1.0203955
H	-3.2117851	-4.7958212	1.0724327
C	-2.6080665	-2.7641473	0.6082974
H	-1.5742985	-3.0431220	0.3522518

S4

75

SCF Energy = -4548.308208183

C	1.6674408	-0.4441330	-2.1255723
C	1.4222394	-1.3239031	-1.0420155
C	1.1177369	-2.6815662	-1.3068822
C	1.0915486	-3.1585487	-2.6225639
C	1.3628137	-2.2843591	-3.6911382
C	1.6482925	-0.9324126	-3.4375465
C	1.4917387	-0.7993273	0.3171237
C	2.4643037	-0.0707980	0.9087343
C	3.7984354	0.0503745	0.2592287
C	4.5130783	-1.0935361	-0.1574741
C	5.7638943	-0.9649909	-0.7784701
C	6.3152669	0.3095682	-0.9924561
C	5.6067863	1.4533337	-0.5845161
C	4.3574746	1.3305241	0.0404858
Br	0.9570940	2.8194049	-0.1674751
C	1.0946515	-1.3612664	3.4716586
C	0.0784001	-0.8790916	4.4786339
C	0.9117482	-2.5446566	2.7625620
C	2.3710699	-0.5582521	3.3767078
C	2.2993847	0.5636263	2.2900891
O	1.0970620	1.2649407	2.4740287
H	3.1837370	1.2246280	2.4478941
H	2.5495686	-0.0636160	4.3527910
H	3.2422390	-1.2043531	3.1550362
H	1.7407016	-2.9823517	2.1864471
H	0.0670217	-3.2147626	2.9995339
H	-0.0680687	0.2131996	4.3657002
H	0.4628366	-1.0544175	5.5077445
H	-0.8947663	-1.4018779	4.3877612
H	1.0003685	1.8819816	1.6590788
H	4.0737404	-2.0885530	0.0088455
H	6.3114453	-1.8653058	-1.0969925
H	7.2956619	0.4118978	-1.4825119
H	6.0244771	2.4552460	-0.7676979
H	3.7626603	2.2203980	0.3017479
H	0.9173370	-3.3572803	-0.4607965
H	0.8617354	-4.2168013	-2.8193913
H	1.3380934	-2.6572261	-4.7262466

H	1.8383634	-0.2439783	-4.2738730
H	1.8516590	0.6187561	-1.9010861
Pd	-0.1395958	-1.0878610	1.4110347
P	-1.6843392	-0.2065981	-0.0732881
C	-2.4083417	1.3803744	0.4570519
C	-1.9852776	1.9462007	1.6746670
H	-1.1795906	1.4609285	2.2457088
C	-2.5560720	3.1467738	2.1202856
H	-2.2089794	3.5958153	3.0624672
C	-3.5379759	3.7889950	1.3488906
H	-3.9736693	4.7393283	1.6929323
C	-3.9525438	3.2305287	0.1273981
H	-4.7127700	3.7397425	-0.4840011
C	-3.3900194	2.0269030	-0.3229987
H	-3.7026433	1.5963798	-1.2859117
C	-3.0027523	-1.4634144	0.2348736
C	-4.3090156	-1.1157113	0.6345814
H	-4.5845449	-0.0562641	0.7379101
C	-5.2520536	-2.1202392	0.9065286
H	-6.2688055	-1.8392909	1.2204464
C	-4.9037831	-3.4750748	0.7808622
H	-5.6469034	-4.2578649	0.9954167
C	-3.6009864	-3.8292333	0.3889868
H	-3.3196203	-4.8889784	0.2947845
C	-2.6513386	-2.8310531	0.1274447
H	-1.6230869	-3.1050104	-0.1577865
C	-1.5475144	-0.0877365	-1.8928073
C	-1.8882130	-1.1672590	-2.7319618
H	-2.2531906	-2.1124343	-2.3071602
C	-1.7757282	-1.0302342	-4.1229720
H	-2.0404169	-1.8766779	-4.7741782
C	-1.3338923	0.1809795	-4.6808761
H	-1.2540009	0.2856059	-5.7738104
C	-0.9887500	1.2529557	-3.8420848
H	-0.6257981	2.2002080	-4.2686147
C	-1.0829399	1.1247786	-2.4492239
H	-0.7548274	1.9459916	-1.7855997

Optimized Geometries(MXnb)

R1
 75
 SCF Energy = -4548.327011132

C	-0.4729729	-0.9931025	-2.9168287
C	-1.0686939	-1.2521951	-1.6572436
C	-2.4381620	-1.6108454	-1.6193472
C	-3.1783622	-1.7167626	-2.8046615
C	-2.5753273	-1.4531475	-4.0466172
C	-1.2178760	-1.0916973	-4.0965657
C	-0.2717465	-1.1033781	-0.4278202
C	0.9360861	-1.6511397	-0.1353850
C	1.5089050	-2.6677062	-1.0690422
C	0.7241458	-3.7558317	-1.5177287
C	1.2334848	-4.6871280	-2.4309707
C	2.5430987	-4.5535166	-2.9226426
C	3.3325519	-3.4750670	-2.4929115
C	2.8243430	-2.5400312	-1.5777083
Br	-2.5857423	-1.4728610	2.1624791
C	1.3997690	-3.5652252	2.2303651
C	0.1734991	-4.3378688	1.8259596
C	2.6085233	-4.1502396	2.4065356
C	1.2182911	-2.0749097	2.3995578
C	1.7035693	-1.2833018	1.1510939
O	3.1065211	-1.4034542	1.0115236
H	1.5025482	-0.2106276	1.3545515
H	0.1544191	-1.8282973	2.5896019
H	1.8185469	-1.6944968	3.2514549
H	3.4711198	-3.5812666	2.7908766
H	2.7592634	-5.2260475	2.2232900
H	-0.3796788	-3.8155699	1.0209869
H	-0.5347847	-4.3826489	2.6815134
H	0.4089569	-5.3699302	1.5027141
H	3.2926758	-2.3693346	1.0317473
H	-0.3033160	-3.8630592	-1.1449447
H	0.6010573	-5.5251108	-2.7615870
H	2.9445128	-5.2852747	-3.6401509
H	4.3567326	-3.3536235	-2.8786769
H	3.4392504	-1.6937090	-1.2492650
H	-2.9075271	-1.8006654	-0.6416947
H	-4.2396090	-2.0048351	-2.7563527
H	-3.1626278	-1.5255980	-4.9746164
H	-0.7362397	-0.8792005	-5.0626611
H	0.5915427	-0.7244157	-2.9622600
Pd	-1.1962816	0.0712840	0.8842850
P	-0.2373501	1.8447653	-0.1191869
C	-0.7813520	3.3221552	0.8220194
C	-1.0576441	4.5498208	0.1875287
H	-0.9547873	4.6369353	-0.9043759
C	-1.4697963	5.6520579	0.9517863

H	-1.6875621	6.6094334	0.4547076
C	-1.6085104	5.5348240	2.3457997
H	-1.9367118	6.4010092	2.9399705
C	-1.3367808	4.3111255	2.9806181
H	-1.4518168	4.2136321	4.0703934
C	-0.9275620	3.2043707	2.2214445
H	-0.7211258	2.2379890	2.7120313
C	1.5857143	1.9763037	-0.1940668
C	2.3061058	1.1533700	-1.0877301
H	1.7700620	0.4875606	-1.7763110
C	3.7066710	1.1730697	-1.0844918
H	4.2583208	0.5259640	-1.7820718
C	4.4017648	2.0014493	-0.1889315
H	5.5019120	2.0049895	-0.1821902
C	3.6893114	2.8197085	0.7020079
H	4.2281617	3.4716575	1.4058428
C	2.2861021	2.8111742	0.7013433
H	1.7324845	3.4546030	1.4004030
C	-0.8408387	2.1116792	-1.8244079
C	-2.1798241	1.7524908	-2.0900806
H	-2.7947517	1.3205202	-1.2850676
C	-2.7048482	1.9091637	-3.3780534
H	-3.7427156	1.6096476	-3.5826162
C	-1.8968658	2.4183308	-4.4095317
H	-2.3054213	2.5249699	-5.4257813
C	-0.5669160	2.7832077	-4.1466153
H	0.0659015	3.1843386	-4.9526756
C	-0.0358414	2.6344358	-2.8548413
H	1.0074090	2.9157358	-2.6505473

R2

75

SCF Energy = -4548.325584991

C	0.9488272	-0.7999505	-2.7601126
C	-0.2309964	-1.0310193	-2.0090645
C	-1.4650803	-1.1504501	-2.6973094
C	-1.5139338	-1.0306366	-4.0921536
C	-0.3391722	-0.7814017	-4.8257996
C	0.8905401	-0.6745064	-4.1540801
C	-0.1570888	-1.0711916	-0.5420106
C	0.6904835	-1.7713876	0.2467422
C	1.5505417	-2.8242612	-0.3678945
C	0.9647108	-3.8662146	-1.1219006
C	1.7582016	-4.8609413	-1.7062908
C	3.1554936	-4.8389894	-1.5475384
C	3.7514122	-3.8051616	-0.8090397

C	2.9577139	-2.8035081	-0.2254348
Br	-3.3733708	-1.3397922	0.6163432
C	-0.1218739	-4.0190974	2.1307266
C	1.1535731	-4.7388322	2.4979864
C	-1.1300770	-4.6399100	1.4828991
C	-0.2378286	-2.5561927	2.4982665
C	0.7164491	-1.5801617	1.7667016
O	2.0393279	-1.5777201	2.3073790
H	0.3266274	-0.5577842	1.9664981
H	-1.2714819	-2.2157201	2.2879040
H	-0.0496271	-2.4131638	3.5860851
H	-2.0437597	-4.0924213	1.2011368
H	-1.0613701	-5.7046550	1.2065065
H	1.4342108	-4.5574253	3.5574191
H	2.0051161	-4.3950341	1.8669533
H	1.0706698	-5.8314694	2.3386671
H	2.4042644	-2.4763759	2.1885901
H	-0.1285677	-3.8890200	-1.2263663
H	1.2818236	-5.6657454	-2.2866723
H	3.7774937	-5.6240697	-2.0037573
H	4.8456140	-3.7688653	-0.6925625
H	3.4271051	-1.9765708	0.3215987
H	-2.3804780	-1.3299039	-2.1127781
H	-2.4792291	-1.1288847	-4.6116955
H	-0.3826656	-0.6745541	-5.9204369
H	1.8160310	-0.4863377	-4.7192362
H	1.9093296	-0.7211652	-2.2343290
Pd	-1.4947877	0.1611862	0.2502883
P	-0.0564674	1.8907595	0.0054620
C	0.2316296	2.8049445	1.5680142
C	1.2992078	3.7178422	1.7009123
H	1.9969692	3.8700939	0.8637294
C	1.4741837	4.4182143	2.9039871
H	2.3097475	5.1269872	3.0066814
C	0.5898431	4.2105910	3.9769374
H	0.7337315	4.7575201	4.9210106
C	-0.4705160	3.2978258	3.8492390
H	-1.1575034	3.1248382	4.6909602
C	-0.6485186	2.5935088	2.6487947
H	-1.4645660	1.8583562	2.5479147
C	1.6301253	1.6653684	-0.6742130
C	1.9919511	2.1702699	-1.9380168
H	1.2648399	2.7422303	-2.5309975
C	3.2789872	1.9335396	-2.4477892
H	3.5520010	2.3276404	-3.4381499
C	4.2074975	1.1933221	-1.7002906

H	5.2145921	1.0040292	-2.1013913
C	3.8489761	0.6964175	-0.4343790
H	4.5767766	0.1246610	0.1602922
C	2.5652706	0.9235737	0.0808621
H	2.3039027	0.5111566	1.0663906
C	-0.8549217	3.0832436	-1.1395794
C	-1.3761418	2.5687473	-2.3492853
H	-1.3072654	1.4911278	-2.5651301
C	-1.9828938	3.4330688	-3.2708911
H	-2.3818479	3.0268269	-4.2122920
C	-2.0920269	4.8058558	-2.9863782
H	-2.5783136	5.4807368	-3.7069558
C	-1.5889339	5.3142393	-1.7776795
H	-1.6810582	6.3867519	-1.5487350
C	-0.9678221	4.4576733	-0.8537911
H	-0.5748332	4.8573040	0.0925000

R3

75

SCF Energy = -4548.324308437

C	-0.4879848	2.4669046	-1.7802026
C	-1.0717938	1.9361655	-0.6025750
C	-1.5398595	2.8350325	0.3886273
C	-1.4324894	4.2185135	0.1985299
C	-0.8470680	4.7333322	-0.9724436
C	-0.3773921	3.8511875	-1.9600640
C	-1.1445539	0.4738774	-0.4355312
C	-1.6213036	-0.4228666	-1.3367723
C	-2.4034437	0.0634831	-2.5138737
C	-3.5861271	0.8134672	-2.3235749
C	-4.3274347	1.2805498	-3.4172114
C	-3.9056785	1.0042452	-4.7290520
C	-2.7297581	0.2662874	-4.9353394
C	-1.9827513	-0.1976468	-3.8401471
Br	-1.8690313	0.4370570	3.2713283
C	-3.1846968	-2.2769250	0.7036980
C	-4.1575867	-1.1454207	0.8950206
C	-2.6260695	-2.9355793	1.7416585
C	-2.7882553	-2.6254167	-0.7177531
C	-1.4808254	-1.9329298	-1.1674929
O	-0.9631725	-2.5641901	-2.3447449
H	-0.7236338	-2.1161924	-0.3811003
H	-2.5981824	-3.7144383	-0.8082829
H	-3.5992493	-2.3658479	-1.4337823
H	-1.9188528	-3.7646609	1.5741089
H	-2.8427308	-2.6542641	2.7827306

H	-5.0972588	-1.3318447	0.3317488
H	-3.7278306	-0.1987402	0.5063803
H	-4.3951318	-0.9828718	1.9619528
H	-1.6331413	-2.4478631	-3.0486147
H	-3.9155612	1.0318915	-1.2979539
H	-5.2431922	1.8658663	-3.2434252
H	-4.4880759	1.3709598	-5.5877725
H	-2.3783567	0.0623179	-5.9585847
H	-1.0325295	-0.7213950	-4.0096044
H	-1.9787809	2.4299454	1.3134978
H	-1.8068124	4.9022372	0.9755911
H	-0.7562057	5.8212994	-1.1133624
H	0.0827592	4.2419751	-2.8803860
H	-0.1270664	1.7774572	-2.5541841
Pd	-0.4407909	-0.0404945	1.3431957
P	1.5332931	-0.4710071	0.3672150
C	2.7868963	0.2518895	1.5011058
C	2.4672820	1.4608890	2.1572402
H	1.4725782	1.9121175	2.0072094
C	3.4064679	2.0662073	3.0055263
H	3.1517588	3.0069009	3.5160147
C	4.6585944	1.4633824	3.2132419
H	5.3904248	1.9332327	3.8876781
C	4.9728132	0.2540743	2.5698071
H	5.9495890	-0.2238297	2.7391269
C	4.0415318	-0.3533545	1.7134580
H	4.2863961	-1.3036133	1.2165303
C	1.9399660	-2.2554792	0.2720456
C	1.2587645	-3.1294322	1.1452512
H	0.4791491	-2.7261828	1.8126821
C	1.5568167	-4.4994064	1.1417055
H	1.0182239	-5.1763388	1.8215848
C	2.5316433	-5.0045628	0.2644721
H	2.7589040	-6.0812773	0.2553925
C	3.2109039	-4.1368226	-0.6070108
H	3.9711252	-4.5317775	-1.2977536
C	2.9195865	-2.7635737	-0.6055261
H	3.4458710	-2.0868171	-1.2946525
C	1.9642070	0.2094656	-1.2775951
C	2.6521039	1.4345602	-1.3817055
H	2.9916933	1.9541575	-0.4743518
C	2.9016036	1.9967912	-2.6438103
H	3.4358633	2.9558567	-2.7147858
C	2.4663801	1.3414306	-3.8057478
H	2.6617979	1.7821470	-4.7949621
C	1.7757330	0.1206560	-3.7016980

H	1.4313957	-0.3957243	-4.6105288
C	1.5155645	-0.4465052	-2.4455440
H	0.9468859	-1.3875181	-2.3832826

R4

75

SCF Energy = -4548.324727949

C	-0.7222347	-0.7660744	-2.8260815
C	-1.2442205	0.1393449	-1.8683751
C	-1.7560101	1.3823914	-2.3184776
C	-1.7495118	1.7002406	-3.6826589
C	-1.2234175	0.7958373	-4.6227180
C	-0.7127187	-0.4384940	-4.1872426
C	-1.2144693	-0.2266739	-0.4412964
C	-1.6237542	-1.3941257	0.1158060
C	-2.4211332	-2.3539020	-0.7034997
C	-3.6178000	-1.9278146	-1.3242264
C	-4.3826734	-2.8127783	-2.0954832
C	-3.9715607	-4.1470066	-2.2603119
C	-2.7827728	-4.5833486	-1.6550826
C	-2.0115628	-3.6955273	-0.8868382
Br	-2.1286704	2.9616304	1.0210384
C	-3.3760722	-0.4666859	2.5649087
C	-2.7388426	0.4440385	3.5815593
C	-4.4454447	-0.1027348	1.8293911
C	-2.7152063	-1.8143378	2.3838711
C	-1.3956640	-1.7428348	1.5834857
O	-0.6498154	-2.9587972	1.7503220
H	-0.7518977	-0.9503786	2.0146170
H	-2.4560468	-2.2527035	3.3722775
H	-3.4025299	-2.5211956	1.8709054
H	-4.8929775	-0.7922452	1.0965504
H	-4.8909444	0.8989595	1.9254829
H	-1.6759525	0.6418815	3.3229728
H	-2.7475597	-0.0235622	4.5905502
H	-3.2420589	1.4267511	3.6296749
H	-1.2552407	-3.6931765	1.5258491
H	-3.9344512	-0.8834658	-1.1926771
H	-5.3096028	-2.4583178	-2.5716115
H	-4.5731543	-4.8422269	-2.8651709
H	-2.4411486	-5.6207638	-1.7939674
H	-1.0527904	-4.0300854	-0.4678151
H	-2.1556036	2.0927944	-1.5785128
H	-2.1579147	2.6669140	-4.0147783
H	-1.2114208	1.0539521	-5.6927949
H	-0.2989760	-1.1556638	-4.9124512

H	-0.3299954	-1.7334444	-2.4879987
Pd	-0.4367819	1.2548011	0.6214591
P	1.5716087	0.2400746	0.4816611
C	2.7624385	1.5941751	0.1257700
C	4.0554781	1.6278159	0.6842433
H	4.3757395	0.8373018	1.3787854
C	4.9286360	2.6775422	0.3592212
H	5.9362169	2.7044984	0.8010449
C	4.5181243	3.6925688	-0.5218233
H	5.2050536	4.5157406	-0.7701430
C	3.2274469	3.6630323	-1.0768315
H	2.8982646	4.4610239	-1.7589369
C	2.3463355	2.6213807	-0.7502721
H	1.3244280	2.6007203	-1.1639536
C	2.1485017	-0.5129908	2.0500555
C	1.5686035	-0.0609154	3.2533206
H	0.7691858	0.6972372	3.2154941
C	1.9984911	-0.5810844	4.4823321
H	1.5365014	-0.2274755	5.4160778
C	3.0074442	-1.5583425	4.5165453
H	3.3387340	-1.9738441	5.4802140
C	3.5889157	-2.0105322	3.3200767
H	4.3770618	-2.7781619	3.3450092
C	3.1639854	-1.4907313	2.0875487
H	3.6135927	-1.8527508	1.1513221
C	1.9177516	-1.0219491	-0.7996827
C	1.4993357	-2.3542067	-0.5862472
H	1.0053748	-2.6414347	0.3560473
C	1.6915133	-3.3099277	-1.5946921
H	1.3672388	-4.3480490	-1.4265530
C	2.2853691	-2.9486774	-2.8173355
H	2.4275821	-3.7031036	-3.6057752
C	2.6911337	-1.6222515	-3.0303417
H	3.1495235	-1.3292656	-3.9865541
C	2.5085286	-0.6586590	-2.0255540
H	2.8243246	0.3799098	-2.1992739

S1

75

SCF Energy = -4548.309690220

C	-0.4469101	1.8876687	-2.2690489
C	-1.3790947	1.3636012	-1.3394668
C	-2.7447527	1.7252419	-1.4930708
C	-3.1680649	2.5229360	-2.5632219
C	-2.2342502	2.9931900	-3.5015833
C	-0.8729105	2.6768414	-3.3424559

C	-1.0361485	0.5559051	-0.1619781
C	-1.5801477	-0.6106097	0.2886926
C	-1.9294539	-1.6885277	-0.6913873
C	-2.6312669	-1.4975981	-1.9036239
C	-2.7793602	-2.5428241	-2.8278432
C	-2.2237554	-3.8073071	-2.5761918
C	-1.5126224	-4.0123766	-1.3819900
C	-1.3700617	-2.9725420	-0.4554111
Br	-1.2892510	2.9801808	1.9746096
C	-4.2245462	-1.7808933	1.3761217
C	-5.1666984	-1.1208969	0.4053754
C	-4.2120401	-3.1148920	1.5739314
C	-3.2789814	-0.8666305	2.1336444
C	-1.7658375	-0.9764024	1.7736892
O	-1.0302713	-0.2290497	2.7177714
H	-1.4586425	-2.0302698	1.9285395
H	-3.5679062	0.1972538	1.9966879
H	-3.3301942	-1.0774369	3.2218643
H	-3.5238343	-3.5833436	2.2961649
H	-4.8751615	-3.7868556	1.0074652
H	-4.6047258	-0.5155890	-0.3359690
H	-5.8460320	-0.4173376	0.9346674
H	-5.7821138	-1.8558271	-0.1480669
H	-1.3024987	0.7219467	2.6597122
H	-3.0624698	-0.5173075	-2.1369832
H	-3.3398468	-2.3608708	-3.7577353
H	-2.3410248	-4.6240945	-3.3042304
H	-1.0549373	-4.9900862	-1.1675476
H	-0.7788642	-3.1500726	0.4533176
H	-3.4623190	1.3880256	-0.7315155
H	-4.2318568	2.7885359	-2.6578250
H	-2.5626324	3.6218870	-4.3430998
H	-0.1297624	3.0550800	-4.0603159
H	0.6198835	1.6733584	-2.1473063
C	3.8062773	2.0192667	0.7054315
C	3.6137257	0.6233540	0.6214135
C	4.6875472	-0.2483559	0.8912561
C	5.9437292	0.2756775	1.2324064
C	6.1351727	1.6665726	1.3053720
C	5.0659465	2.5388395	1.0412004
P	1.9426086	0.0238237	0.1527289
C	2.0310532	-0.2011293	-1.6659075
C	2.9561127	0.5194838	-2.4483234
C	2.8756931	0.4711428	-3.8496666
C	1.8780577	-0.2948825	-4.4761640
C	0.9672300	-1.0287127	-3.6970727

C	1.0407570	-0.9850421	-2.2989709
Pd	0.3481649	1.4927509	0.9159328
C	1.8541740	-1.6988852	0.7822373
C	2.2985927	-2.7970591	0.0145677
C	2.2117391	-4.0975250	0.5340377
C	1.6883752	-4.3101724	1.8209727
C	1.2616708	-3.2159520	2.5921267
C	1.3444811	-1.9121021	2.0783061
H	2.6976786	-2.6377327	-0.9972212
H	2.5498143	-4.9502029	-0.0739574
H	1.6110634	-5.3322905	2.2218476
H	0.8455170	-3.3749749	3.5983247
H	0.9499129	-1.0630540	2.6556738
H	3.7318311	1.1291593	-1.9617046
H	3.5986348	1.0384492	-4.4553152
H	1.8125366	-0.3215376	-5.5743424
H	0.1790061	-1.6310137	-4.1721622
H	0.3107550	-1.5488404	-1.7030794
H	4.5359105	-1.3368176	0.8397717
H	6.7797565	-0.4074234	1.4460741
H	7.1214117	2.0722216	1.5771789
H	5.2094982	3.6278491	1.1049870
H	2.9584132	2.6970469	0.5045058

S2

75

SCF Energy = -4548.312853955

C	-1.9904918	-0.4536652	-2.1241148
C	-1.3435821	-1.3946903	-1.2835712
C	-1.6099252	-2.7728458	-1.5042941
C	-2.4273325	-3.1930837	-2.5614406
C	-3.0175646	-2.2460644	-3.4138985
C	-2.8010224	-0.8750167	-3.1820950
C	-0.5098284	-1.0531775	-0.1260795
C	0.6711012	-1.5899923	0.2898468
C	1.7286292	-1.9363046	-0.7132847
C	1.5680802	-2.7716911	-1.8399966
C	2.5966799	-2.9158859	-2.7830542
C	3.8156457	-2.2351868	-2.6274119
C	3.9963394	-1.4061892	-1.5084393
C	2.9701218	-1.2623705	-0.5644004
Br	-2.7929822	-1.3075934	2.1712162
C	1.4247318	-4.3637856	1.2440896
C	2.9307170	-4.4283694	1.2303981
C	0.6629280	-5.2323157	0.5450539
C	0.7922550	-3.3014129	2.1117445

C	1.0818175	-1.8089236	1.7593355
O	0.4717423	-1.0047347	2.7464327
H	2.1705838	-1.6175776	1.8533039
H	-0.3122726	-3.4145928	2.1043825
H	1.1322248	-3.4243728	3.1642534
H	-0.4370526	-5.1908052	0.5913043
H	1.1133454	-6.0189329	-0.0809659
H	3.3274704	-4.5462369	2.2621627
H	3.3712000	-3.4939467	0.8238714
H	3.3007587	-5.2701898	0.6145575
H	-0.4953696	-1.2184491	2.7698225
H	0.6325760	-3.3239336	-1.9771749
H	2.4421524	-3.5782513	-3.6486728
H	4.6187292	-2.3528302	-3.3705529
H	4.9388550	-0.8557013	-1.3673585
H	3.1170360	-0.5820817	0.2864323
H	-1.1808552	-3.5037910	-0.8052427
H	-2.6156841	-4.2671878	-2.7101668
H	-3.6642698	-2.5726188	-4.2424416
H	-3.2760424	-0.1228291	-3.8295517
H	-1.8562181	0.6178746	-1.9412427
Pd	-1.4002731	0.3283615	0.9991110
P	-0.0165694	1.9463460	0.1337531
C	1.7428417	1.9136560	0.6557887
C	2.7720418	2.4065635	-0.1752974
H	2.5322008	2.8107984	-1.1691717
C	4.1059060	2.3596569	0.2575025
H	4.9048508	2.7368884	-0.3986174
C	4.4202538	1.8266441	1.5196303
H	5.4684981	1.7810550	1.8521224
C	3.3946652	1.3477457	2.3519696
H	3.6337665	0.9208790	3.3376629
C	2.0576928	1.3905599	1.9253432
H	1.2638394	0.9512470	2.5477436
C	-0.6370142	3.6040535	0.6224623
C	0.2162953	4.7023883	0.8486668
H	1.3050174	4.5803826	0.7482234
C	-0.3258487	5.9453926	1.2096573
H	0.3432709	6.8004908	1.3894179
C	-1.7165737	6.0993514	1.3457129
H	-2.1362295	7.0755205	1.6322079
C	-2.5703850	5.0054791	1.1255200
H	-3.6588187	5.1193929	1.2393113
C	-2.0324814	3.7589960	0.7704038
H	-2.6950502	2.8916412	0.6052151
C	0.0997889	2.0203160	-1.6957328

C	0.8526199	1.0273383	-2.3614551
H	1.4530403	0.3069679	-1.7896898
C	0.8195632	0.9409382	-3.7589115
H	1.3987010	0.1519320	-4.2608205
C	0.0388690	1.8407146	-4.5047025
H	0.0049384	1.7643483	-5.6019700
C	-0.6962077	2.8408892	-3.8464249
H	-1.2995505	3.5554810	-4.4266416
C	-0.6673219	2.9346354	-2.4453293
H	-1.2523473	3.7127500	-1.9329213

S3

75

SCF Energy = -4548.330436499

C	-1.1080454	-0.5678198	-2.4444733
C	-1.3253599	-0.9793852	-1.1061965
C	-2.6542081	-1.2528168	-0.6958182
C	-3.7212137	-1.1087189	-1.5925090
C	-3.4911784	-0.6798110	-2.9119752
C	-2.1775662	-0.4155327	-3.3343360
C	-0.1983868	-1.0614847	-0.1567203
C	0.9858622	-1.7053693	-0.3276978
C	1.1957197	-2.5599431	-1.5339031
C	0.2171091	-3.4898666	-1.9549469
C	0.4172840	-4.2813139	-3.0931586
C	1.6051923	-4.1695967	-3.8362437
C	2.5934544	-3.2621190	-3.4217600
C	2.3935137	-2.4691129	-2.2814782
Br	-1.6387659	-1.6573014	2.9721845
C	1.6516435	-3.6827725	2.0759309
C	0.4409832	-4.3772221	1.5109245
C	1.8266398	-3.5146571	3.4073050
C	2.6315097	-3.0752607	1.0958731
C	2.1825829	-1.6529857	0.6364641
O	2.0218533	-0.8221851	1.7685698
H	3.0280806	-1.2087700	0.0654721
H	3.6230511	-2.9547491	1.5761433
H	2.7606843	-3.7233835	0.2062543
H	2.7162274	-3.0021327	3.8080075
H	1.0914604	-3.8938036	4.1336942
H	0.7296885	-5.1105057	0.7293186
H	-0.2352363	-3.6378909	1.0337849
H	-0.1396653	-4.8918805	2.2992587
H	1.4894976	-1.3428654	2.4172112
H	-0.7101205	-3.5885899	-1.3742389
H	-0.3606792	-4.9969530	-3.3999216

H	1.7625418	-4.7926038	-4.7296605
H	3.5308420	-3.1680882	-3.9916401
H	3.1707921	-1.7551405	-1.9755712
H	-2.8309897	-1.5671444	0.3445078
H	-4.7453259	-1.3285503	-1.2541617
H	-4.3332792	-0.5534249	-3.6092228
H	-1.9834228	-0.0832470	-4.3652437
H	-0.0808059	-0.3834704	-2.7854583
Pd	-0.6164003	-0.0241092	1.4790303
P	0.2673816	1.7743836	0.4473204
C	-0.7887682	2.4888907	-0.8633024
C	-0.2917130	3.3158011	-1.8921455
H	0.7784365	3.5679962	-1.9294061
C	-1.1640790	3.8040588	-2.8777669
H	-0.7733524	4.4433797	-3.6839157
C	-2.5297295	3.4747286	-2.8381117
H	-3.2073549	3.8495954	-3.6201692
C	-3.0291613	2.6644027	-1.8048817
H	-4.0947915	2.3952683	-1.7744436
C	-2.1624001	2.1718782	-0.8205615
H	-2.5348671	1.5082648	-0.0242556
C	0.4293113	3.0689573	1.7373292
C	0.8322619	2.6586255	3.0283382
H	1.0367890	1.5922587	3.2191755
C	0.9651722	3.6050639	4.0554105
H	1.2788550	3.2805584	5.0588240
C	0.6855280	4.9589264	3.8038673
H	0.7814582	5.6997475	4.6119958
C	0.2732947	5.3663000	2.5234370
H	0.0467719	6.4254292	2.3281448
C	0.1438707	4.4262364	1.4893981
H	-0.1871929	4.7439294	0.4896176
C	1.9409915	1.6184683	-0.2842831
C	2.0905708	1.1606701	-1.6098789
H	1.2032263	0.9906647	-2.2330496
C	3.3687763	0.9261218	-2.1376947
H	3.4704211	0.5783281	-3.1764519
C	4.5083272	1.1270772	-1.3407941
H	5.5109862	0.9363209	-1.7522404
C	4.3625663	1.5757220	-0.0170841
H	5.2501935	1.7339068	0.6135147
C	3.0868506	1.8238375	0.5100967
H	2.9822934	2.1670337	1.5483708

S4
75

SCF Energy = -4548.326599873

C	-1.0609715	-0.4950362	-2.4397624
C	-1.2447221	-0.9808505	-1.1214537
C	-2.5614627	-1.2850190	-0.6948902
C	-3.6493205	-1.1100808	-1.5608272
C	-3.4510637	-0.6205585	-2.8634240
C	-2.1500380	-0.3167006	-3.2994576
C	-0.0937901	-1.1184343	-0.2076488
C	1.0717237	-1.7767732	-0.4405901
C	1.1971051	-2.6150427	-1.6722072
C	0.1669131	-3.4987158	-2.0692131
C	0.2842233	-4.2642250	-3.2362034
C	1.4367598	-4.1690923	-4.0351550
C	2.4737038	-3.3053625	-3.6478757
C	2.3575866	-2.5406210	-2.4768513
Br	-1.8157986	-1.4204252	3.0843503
C	1.2890868	-3.6487359	2.0348274
C	1.4680118	-3.2496780	3.4779864
C	0.1739106	-4.2645035	1.5898327
C	2.4133474	-3.2890037	1.0876340
C	2.2846330	-1.8486988	0.4927048
O	2.3637244	-0.8590790	1.4955170
H	3.1850971	-1.6868240	-0.1396561
H	3.3919425	-3.3276678	1.6105301
H	2.4567915	-4.0053519	0.2425274
H	0.0726353	-4.5686698	0.5367795
H	-0.6745497	-4.4663417	2.2610246
H	1.7660020	-2.1847597	3.5600196
H	2.2919693	-3.8364252	3.9418437
H	0.5440085	-3.4014460	4.0664179
H	1.4498738	-0.7514376	1.8755976
H	-0.7347829	-3.5785816	-1.4470379
H	-0.5311897	-4.9459557	-3.5220601
H	1.5287135	-4.7710056	-4.9518355
H	3.3832681	-3.2235328	-4.2627927
H	3.1734638	-1.8615595	-2.1904627
H	-2.7152619	-1.6525814	0.3314611
H	-4.6635062	-1.3565461	-1.2114887
H	-4.3087492	-0.4736676	-3.5372179
H	-1.9819786	0.0693344	-4.3158676
H	-0.0460752	-0.2681476	-2.7934179
Pd	-0.5194247	-0.1427862	1.4799524
P	0.4103040	1.6593051	0.4913565
C	0.4272386	2.9459807	1.7974358
C	0.7374867	2.5591450	3.1194567
H	0.9498969	1.5014190	3.3444924

C	0.7653484	3.5189929	4.1421932
H	1.0042187	3.2120825	5.1712393
C	0.4772594	4.8631903	3.8519139
H	0.4915342	5.6142814	4.6560943
C	0.1621653	5.2485724	2.5373675
H	-0.0686724	6.3005022	2.3111202
C	0.1355516	4.2944607	1.5089615
H	-0.1177582	4.5924335	0.4807379
C	2.1049377	1.6585703	-0.1980705
C	2.3650680	1.0029821	-1.4203767
H	1.5460324	0.5330869	-1.9784344
C	3.6718423	0.9492960	-1.9253267
H	3.8606393	0.4471487	-2.8860435
C	4.7310373	1.5332871	-1.2103928
H	5.7570469	1.4836367	-1.6049640
C	4.4746221	2.1839866	0.0072686
H	5.2989313	2.6441634	0.5723959
C	3.1677688	2.2512017	0.5118052
H	2.9749029	2.7583665	1.4676327
C	-0.6766058	2.3195509	-0.8230491
C	-0.1900390	2.9770898	-1.9695781
H	0.8907808	3.1318232	-2.0994544
C	-1.0895657	3.4232813	-2.9517240
H	-0.7068526	3.9301505	-3.8504454
C	-2.4693243	3.2195723	-2.7906399
H	-3.1695335	3.5588549	-3.5688420
C	-2.9567969	2.5767274	-1.6394247
H	-4.0354338	2.4046886	-1.5140450
C	-2.0655469	2.1261282	-0.6589489
H	-2.4380577	1.5912447	0.2292613

Optimized Geometries (BXnc)

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R1
75
SCF Energy = -4548.338894608
C    -1.1655986    2.4014617   -0.4483549
C    -1.0215485    1.1681360   -1.1357378
C    -2.1947491    0.5725807   -1.6627296
C    -3.4513404    1.1643854   -1.4821957
C    -3.5721527    2.3850030   -0.7976166
C    -2.4186495    3.0065465   -0.2923733
C     0.3152153    0.5472003   -1.2266883

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C	0.8971215	-0.0283725	-2.3140060
C	0.2737066	-0.0886752	-3.6618711
C	0.3318581	-1.2858684	-4.4152226
C	-0.2741945	-1.3756874	-5.6774898
C	-0.9411243	-0.2653086	-6.2214438
C	-0.9902077	0.9363994	-5.4933363
C	-0.3886983	1.0241047	-4.2308266
Br	1.6266467	1.5428172	2.9439405
C	2.8125198	1.8685744	-1.1362276
C	2.1354130	3.0798021	-1.7287435
C	3.2222788	1.8630481	0.1859478
C	3.2504356	0.8021657	-2.1239276
C	2.3561808	-0.4648968	-2.2177841
O	2.6782240	-1.2825539	-1.1007943
H	2.6402374	-0.9894632	-3.1592815
H	3.2935046	1.2535566	-3.1358995
H	4.2703852	0.4474206	-1.8702941
H	3.9142632	1.0913887	0.5564719
H	3.0986632	2.7538177	0.8187392
H	1.2728519	2.7918266	-2.3615779
H	2.8555258	3.6097904	-2.3901363
H	1.7914895	3.7893789	-0.9528487
H	1.9261606	-1.8880746	-0.9460876
H	0.8418850	-2.1634258	-3.9899926
H	-0.2245821	-2.3203905	-6.2407500
H	-1.4142426	-0.3330490	-7.2127316
H	-1.4987202	1.8165576	-5.9157135
H	-0.4335069	1.9668156	-3.6667461
H	-2.1187107	-0.3566827	-2.2430481
H	-4.3462969	0.6669610	-1.8856571
H	-4.5609746	2.8464214	-0.6565497
H	-2.4949895	3.9629826	0.2466526
H	-0.2715980	2.8741799	-0.0145061
Pd	1.2739011	0.7419454	0.5563832
P	0.0400467	-1.0422607	1.2985181
C	-1.7364039	-0.7118993	1.5755500
C	-2.0749717	0.5584706	2.0864471
H	-1.2740924	1.2849982	2.2967430
C	-3.4190758	0.8771292	2.3218800
H	-3.6800185	1.8725703	2.7102374
C	-4.4279520	-0.0614933	2.0486519
H	-5.4833119	0.1980228	2.2224088
C	-4.0901865	-1.3318433	1.5538492
H	-4.8774158	-2.0725084	1.3465713
C	-2.7464341	-1.6616264	1.3197399
H	-2.4841336	-2.6574867	0.9347708

C	0.0917678	-2.5239138	0.1962296
C	0.9538479	-3.6088599	0.4718680
H	1.5476832	-3.6166173	1.3964481
C	1.0649065	-4.6746630	-0.4364142
H	1.7480823	-5.5071942	-0.2111435
C	0.3070940	-4.6828698	-1.6185231
H	0.3944802	-5.5213213	-2.3258067
C	-0.5682111	-3.6171042	-1.8896347
H	-1.1732756	-3.6122658	-2.8082877
C	-0.6686611	-2.5429440	-0.9948400
H	-1.3497934	-1.7139925	-1.2137130
C	0.6653406	-1.7358636	2.8769591
C	2.0583458	-1.7830163	3.0938594
H	2.7381232	-1.3280213	2.3585469
C	2.5639168	-2.3851901	4.2537743
H	3.6508816	-2.4167937	4.4211826
C	1.6846979	-2.9219990	5.2108896
H	2.0835668	-3.3803194	6.1285985
C	0.2980127	-2.8625828	5.0010212
H	-0.3935623	-3.2722296	5.7527356
C	-0.2147475	-2.2757736	3.8321173
H	-1.3012465	-2.2280058	3.6683782

R2

75

SCF Energy = -4548.318797620

C	2.4678109	0.7548753	-2.1626642
C	2.0554557	-0.3112123	-1.3247944
C	1.5421071	-1.4873986	-1.9300645
C	1.4462251	-1.5954193	-3.3245469
C	1.8634319	-0.5330627	-4.1429939
C	2.3751332	0.6389537	-3.5547328
C	2.0920221	-0.2031879	0.1428062
C	3.1714397	-0.0854862	0.9452359
C	4.5556223	0.0059525	0.3933551
C	5.0066477	-0.8557240	-0.6338876
C	6.3094685	-0.7529806	-1.1395938
C	7.1984287	0.2063558	-0.6245823
C	6.7717783	1.0598322	0.4056095
C	5.4659075	0.9603836	0.9106054
Br	0.2024597	2.2748779	-0.0627371
C	1.0044567	-1.6334468	2.1177117
C	1.7690614	-2.8515962	1.6527123
C	-0.3993880	-1.6553332	2.0910760
C	1.7345140	-0.6436528	3.0057426
C	3.0927818	-0.1524145	2.4690707

O	4.0782026	-1.0688412	2.9657380
H	3.2732405	0.8646016	2.8998719
H	1.0723879	0.2186797	3.2153134
H	1.9653305	-1.1306286	3.9794485
H	-0.9847670	-1.0484383	2.8012831
H	-0.9219144	-2.5337070	1.6824353
H	1.9449851	-3.5042739	2.5354580
H	2.7617323	-2.5961663	1.2440418
H	1.1939299	-3.4321048	0.9057097
H	4.8962527	-0.9066108	2.4534815
H	4.3206494	-1.6160173	-1.0323285
H	6.6364893	-1.4342321	-1.9399878
H	8.2218731	0.2846439	-1.0214309
H	7.4580635	1.8162690	0.8162721
H	5.1350895	1.6495988	1.7025874
H	1.2193336	-2.3186076	-1.2860151
H	1.0386972	-2.5132363	-3.7744792
H	1.7883872	-0.6157966	-5.2379054
H	2.7012875	1.4760174	-4.1909192
H	2.8432287	1.6759859	-1.6978059
Pd	0.0874541	-0.1687925	0.5778020
P	-2.2056252	-0.0303910	0.0726197
C	-3.1256564	1.4096793	0.7349701
C	-2.4545728	-0.0330859	-1.7515710
C	-3.2322060	-1.4638645	0.6017411
C	-4.2486679	1.9532090	0.0832236
C	-4.9510392	3.0172426	0.6710233
C	-4.5386069	3.5374699	1.9091817
C	-3.4130661	3.0004124	2.5571951
C	-2.7016515	1.9453775	1.9680710
H	-4.5671218	1.5537876	-0.8907863
H	-5.8235786	3.4457010	0.1549346
H	-5.0900463	4.3732956	2.3659808
H	-3.0759240	3.4176932	3.5178913
H	-1.7946452	1.5455543	2.4461858
C	-3.6666407	-0.5035573	-2.3065907
C	-3.8525779	-0.5016900	-3.6970185
C	-2.8308584	-0.0381475	-4.5438098
C	-1.6238450	0.4229247	-3.9950107
C	-1.4310138	0.4271566	-2.6051049
H	-4.4616883	-0.8863106	-1.6495136
H	-4.7997900	-0.8688900	-4.1206125
H	-2.9765390	-0.0422678	-5.6349365
H	-0.8125165	0.7776875	-4.6469730
H	-0.4879313	0.7993367	-2.1792369
C	-4.1858498	-1.3654574	1.6325920

C	-4.8667509	-2.5130916	2.0756422
C	-4.6038535	-3.7621708	1.4928640
C	-3.6514092	-3.8651006	0.4619937
C	-2.9651439	-2.7253709	0.0227404
H	-4.4012260	-0.3870554	2.0868863
H	-5.6123326	-2.4254833	2.8805276
H	-5.1404643	-4.6581175	1.8396098
H	-3.4419294	-4.8414234	-0.0009394
H	-2.2167355	-2.8070843	-0.7817191

R3

75

SCF Energy = -4548.319139529

C	0.2082874	2.6414696	-1.7001936
C	-0.2993797	1.6093136	-2.5314058
C	-0.9179756	1.9966357	-3.7526261
C	-1.0009180	3.3415877	-4.1287334
C	-0.4824884	4.3481917	-3.2941318
C	0.1196404	3.9880362	-2.0775135
C	-0.2867695	0.1993576	-2.1277724
C	-0.2676397	-0.9095222	-2.9119391
C	0.1818006	-0.9024988	-4.3220267
C	-0.5222019	-1.5851193	-5.3456357
C	-0.0736435	-1.5343757	-6.6750422
C	1.0836779	-0.8114424	-7.0079028
C	1.7998056	-0.1444573	-5.9973042
C	1.3595933	-0.1950224	-4.6693380
Br	2.0987197	-0.0323226	-0.3198772
C	-2.4419863	-0.8216522	-0.9932605
C	-3.2123520	0.1793177	-1.8214556
C	-2.4232714	-0.6904451	0.4027277
C	-2.1012610	-2.1412175	-1.6653991
C	-0.6572988	-2.2253244	-2.2279432
O	-0.6027984	-3.3795628	-3.0449539
H	0.0327803	-2.3300226	-1.3497610
H	-2.2443948	-2.9832792	-0.9580262
H	-2.7888026	-2.3026189	-2.5211315
H	-2.2846863	-1.5768582	1.0423580
H	-2.9558269	0.1483844	0.8775149
H	-2.8166472	0.2617315	-2.8494396
H	-3.2160031	1.1874753	-1.3665147
H	-4.2641191	-0.1761395	-1.8969038
H	0.2403494	-3.3463270	-3.5365879
H	-1.4314006	-2.1471168	-5.0923802
H	-0.6390375	-2.0609008	-7.4595464
H	1.4315968	-0.7732935	-8.0514508

H	2.7154885	0.4134126	-6.2466629
H	1.9223182	0.3080669	-3.8690124
H	-1.3284155	1.2205558	-4.4136786
H	-1.4807959	3.6082526	-5.0830592
H	-0.5536127	5.4061294	-3.5892987
H	0.5274414	4.7636177	-1.4111530
H	0.6889869	2.3651842	-0.7532417
Pd	-0.4032177	-0.0536846	-0.0720273
P	-0.0251779	0.0177263	2.2804350
C	0.6767137	1.5795109	2.9652939
C	1.5171274	2.3818926	2.1662624
H	1.7638229	2.0539353	1.1450037
C	2.0693444	3.5613078	2.6887996
H	2.7244538	4.1778576	2.0549666
C	1.7917212	3.9514183	4.0090704
H	2.2242124	4.8786278	4.4149258
C	0.9609181	3.1521415	4.8118444
H	0.7420136	3.4478549	5.8491817
C	0.4036894	1.9723248	4.2950803
H	-0.2521433	1.3570128	4.9277818
C	1.1049476	-1.3173496	2.8332769
C	1.1144867	-2.5184440	2.0947584
H	0.5089817	-2.5924778	1.1781837
C	1.9120832	-3.5934661	2.5120017
H	1.9186350	-4.5268812	1.9294282
C	2.7165083	-3.4684791	3.6575991
H	3.3519220	-4.3079738	3.9782337
C	2.7196084	-2.2671109	4.3859953
H	3.3579892	-2.1628922	5.2764345
C	1.9141005	-1.1920648	3.9781696
H	1.9231335	-0.2493725	4.5450040
C	-1.5051446	-0.2290175	3.3504418
C	-1.7328646	-1.4311671	4.0476154
H	-0.9731409	-2.2262131	4.0290045
C	-2.9236707	-1.6129339	4.7724505
H	-3.0900755	-2.5555390	5.3156970
C	-3.8920607	-0.5980607	4.8102046
H	-4.8218337	-0.7417086	5.3809410
C	-3.6690738	0.6050846	4.1162311
H	-4.4228977	1.4065086	4.1430669
C	-2.4873686	0.7865540	3.3852693
H	-2.3162617	1.7301060	2.8429963

R4

75

SCF Energy = -4548.331369847

C	1.1637123	-5.5508535	0.4604941
C	0.0951317	-4.6672686	0.1657364
C	-0.9762561	-5.1497181	-0.6234802
C	-0.9765623	-6.4626793	-1.1128291
C	0.0902947	-7.3282255	-0.8160203
C	1.1573623	-6.8666637	-0.0276147
C	0.1070858	-3.2572244	0.6361852
Pd	-0.2143375	-0.2939553	0.3522801
P	-0.3017088	2.1025651	0.1356232
C	-0.1697094	-2.2291108	-0.1929562
Br	2.2200228	-0.2274126	-0.2556841
C	-0.3301764	-2.2060972	-1.6517160
C	0.7058588	-2.6857295	-2.4932229
C	0.6039201	-2.5694424	-3.8837086
C	-0.5269389	-1.9679811	-4.4684911
C	-1.5612485	-1.4883476	-3.6487647
C	-1.4644536	-1.6044132	-2.2549319
C	0.3283392	-2.9480589	2.1192453
O	0.6936609	-4.0645895	2.9064203
C	-0.9782941	-2.2943278	2.6781803
C	-1.2512756	-0.8622855	2.2624261
C	-2.1780692	-0.5436841	1.2446162
C	-0.8126917	0.1827462	3.2642013
H	1.1569789	-2.2140674	2.2184000
H	-0.8806260	-2.3263459	3.7823487
H	-1.8269567	-2.9493313	2.3946097
H	-2.7238589	-1.3629611	0.7505278
H	-2.6702671	0.4405555	1.2398778
H	-1.4031473	0.0620649	4.1996720
H	-0.9663629	1.2144191	2.8981328
H	0.2537287	0.0502545	3.5382229
H	0.1424925	-4.8192101	2.6170828
H	-1.8126532	-4.4732554	-0.8514000
H	-1.8190559	-6.8151474	-1.7274615
H	0.0896299	-8.3603039	-1.1983255
H	2.0014457	-7.5347235	0.2030463
H	2.0068287	-5.1887142	1.0645906
H	-2.2696211	-1.2187801	-1.6129866
H	-2.4457589	-1.0107154	-4.0962929
H	-0.5984218	-1.8720291	-5.5626785
H	1.4194871	-2.9431866	-4.5215458
H	1.5982887	-3.1267418	-2.0286873
C	-0.4746418	2.4765301	-1.6608216
C	1.1253064	3.0985431	0.7172542
C	-1.7405701	2.9739450	0.8795650
C	-1.6005999	3.7929678	2.0189690

C	-2.7350337	4.3368667	2.6437771
C	-4.0180583	4.0733653	2.1381515
C	-4.1649083	3.2602924	1.0004139
C	-3.0360228	2.7081675	0.3783531
H	-0.5970365	4.0109756	2.4134382
H	-2.6119771	4.9776724	3.5301169
H	-4.9047483	4.5035548	2.6275417
H	-5.1668559	3.0533188	0.5946928
H	-3.1555297	2.0761184	-0.5155596
C	-1.1490769	3.6309769	-2.1170764
C	-1.2672722	3.8810089	-3.4928993
C	-0.7170650	2.9826098	-4.4233622
C	-0.0439338	1.8354339	-3.9732751
C	0.0798853	1.5802495	-2.5993143
H	-1.5954856	4.3299582	-1.3942689
H	-1.7956349	4.7823425	-3.8393771
H	-0.8166763	3.1780578	-5.5020663
H	0.3841879	1.1203355	-4.6909750
H	0.6190018	0.6858900	-2.2513117
C	1.8822138	2.6066221	1.7993040
C	2.9399913	3.3674963	2.3195638
C	3.2576953	4.6120920	1.7508837
C	2.5155283	5.0961542	0.6600066
C	1.4502456	4.3429885	0.1431692
H	1.6519535	1.6142264	2.2122362
H	3.5304362	2.9766842	3.1618262
H	4.0948857	5.2032595	2.1522699
H	2.7706606	6.0650624	0.2045290
H	0.8761992	4.7192242	-0.7165195

S1

75

SCF Energy = -4548.341425160

C	-2.2996591	1.0062732	-2.5926963
C	-1.6766063	-0.2058107	-2.1971339
C	-2.4777496	-1.2183595	-1.6075269
C	-3.8545000	-1.0276129	-1.4229173
C	-4.4570145	0.1760933	-1.8216126
C	-3.6740722	1.1891223	-2.4086511
C	-0.2211549	-0.3617511	-2.2860983
C	0.6267210	-0.2661623	-3.3314616
C	0.1627511	-0.0658345	-4.7267527
C	-0.9701122	-0.7368211	-5.2417795
C	-1.4066041	-0.5012188	-6.5528066
C	-0.7212650	0.4084240	-7.3764435
C	0.4083291	1.0791206	-6.8773179

C	0.8499062	0.8423880	-5.5676621
Br	0.2921491	2.1303539	-0.4140058
C	2.0306683	-1.7440767	-0.8575687
C	3.0927320	-1.3931742	0.1591590
C	0.8857495	-2.4897350	-0.4855027
C	2.4742932	-1.6372840	-2.3034858
C	2.1304728	-0.3268618	-3.0768594
O	2.6581552	0.8350750	-2.4653120
H	2.6431072	-0.4225932	-4.0577964
H	3.5797146	-1.7320735	-2.3209104
H	2.0583674	-2.4788198	-2.8928933
H	0.3135966	-3.0057823	-1.2728602
H	0.8167009	-2.9209334	0.5247328
H	3.5077249	-0.3875617	-0.0537119
H	3.9351619	-2.1148811	0.0697557
H	2.7191429	-1.4353573	1.1992337
H	1.9614068	1.2176423	-1.8743394
H	-1.5023443	-1.4570158	-4.6039182
H	-2.2873358	-1.0379571	-6.9378396
H	-1.0650690	0.5920089	-8.4057198
H	0.9481332	1.7986779	-7.5120400
H	1.7176692	1.3890714	-5.1678428
H	-2.0024713	-2.1582998	-1.2915835
H	-4.4581234	-1.8205567	-0.9566641
H	-5.5367648	0.3290454	-1.6728004
H	-4.1423344	2.1356971	-2.7188995
H	-1.6769353	1.8021041	-3.0231829
Pd	0.3076229	-0.4130915	-0.3472777
P	0.0758384	-0.3275691	2.0433684
C	-1.7169061	-0.0893893	2.3944444
C	-2.4954532	0.6484687	1.4770028
H	-2.0284486	1.0719130	0.5745357
C	-3.8623290	0.8503683	1.7192842
H	-4.4563423	1.4210346	0.9907984
C	-4.4645028	0.3189887	2.8711376
H	-5.5383960	0.4749425	3.0556783
C	-3.6935426	-0.4163007	3.7876881
H	-4.1597596	-0.8356006	4.6923351
C	-2.3250544	-0.6206606	3.5532578
H	-1.7287902	-1.2062132	4.2686318
C	0.4915780	-1.8546502	2.9773517
C	1.6171958	-1.9215225	3.8236094
H	2.2064006	-1.0134690	4.0197907
C	1.9808821	-3.1395361	4.4216987
H	2.8598215	-3.1788316	5.0828964
C	1.2250619	-4.2988429	4.1856106

H	1.5101597	-5.2507328	4.6582706
C	0.1001085	-4.2384865	3.3438673
H	-0.4990709	-5.1424744	3.1566391
C	-0.2609747	-3.0274099	2.7367466
H	-1.1424715	-2.9837718	2.0778300
C	0.9385560	0.9863672	2.9898252
C	2.1574376	1.4837306	2.4871927
H	2.5258424	1.1307172	1.5143243
C	2.8768214	2.4439464	3.2146741
H	3.8257374	2.8317592	2.8150471
C	2.3748874	2.9231912	4.4359690
H	2.9345615	3.6844046	5.0005466
C	1.1510096	2.4406271	4.9308296
H	0.7498602	2.8232948	5.8815642
C	0.4327094	1.4736562	4.2111418
H	-0.5295859	1.1037460	4.5950142

S2

75

SCF Energy = -4548.330443648

C	-1.9024475	1.2311906	-3.0886615
C	-1.5813991	0.0713554	-2.3383258
C	-2.6391482	-0.6441280	-1.7235456
C	-3.9698933	-0.2225065	-1.8587728
C	-4.2720011	0.9256617	-2.6095019
C	-3.2313340	1.6475030	-3.2233183
C	-0.1850138	-0.3166045	-2.1123961
C	0.8449022	-0.4044176	-2.9904222
C	0.7037995	-0.2680783	-4.4602769
C	-0.3896343	-0.8402386	-5.1521909
C	-0.5186782	-0.6935771	-6.5396673
C	0.4432255	0.0262832	-7.2695392
C	1.5378746	0.5952061	-6.5970963
C	1.6696810	0.4463436	-5.2086905
Br	0.0752188	2.0996809	-0.2575980
C	0.9088986	-2.4869307	-0.9545615
C	-0.1480485	-3.3082868	-1.6576367
C	0.8980458	-2.3874458	0.4436387
C	2.1499784	-2.1656618	-1.7625270
C	2.2128282	-0.7428713	-2.4156158
O	2.6991748	0.2173746	-1.4857255
H	2.9599875	-0.8108330	-3.2346859
H	3.0550306	-2.2612588	-1.1297184
H	2.2306773	-2.9078400	-2.5841245
H	1.8287860	-2.1622943	0.9892576
H	0.1313902	-2.9227582	1.0256832

H	0.2649273	-4.3243925	-1.8443196
H	-0.4166088	-2.8778489	-2.6409199
H	-1.0661403	-3.4196055	-1.0503928
H	1.9565461	0.8204527	-1.2393498
H	-1.1436478	-1.4067440	-4.5864914
H	-1.3760260	-1.1501813	-7.0577059
H	0.3414257	0.1406302	-8.3593916
H	2.2945906	1.1650299	-7.1580625
H	2.5174032	0.9135372	-4.6843710
H	-2.4018472	-1.5342483	-1.1226951
H	-4.7746995	-0.7923258	-1.3696332
H	-5.3148953	1.2619844	-2.7128406
H	-3.4593011	2.5549420	-3.8031975
H	-1.0864482	1.8097033	-3.5425576
Pd	0.1235494	-0.4241791	-0.0756735
P	-0.0348234	-0.0430490	2.2471367
C	-1.7028830	0.5663803	2.7187244
C	-2.6015747	0.9885954	1.7173562
H	-2.2897006	0.9825901	0.6628646
C	-3.8897931	1.4214790	2.0674157
H	-4.5815893	1.7437582	1.2749045
C	-4.2892013	1.4402155	3.4134331
H	-5.2995575	1.7820947	3.6853749
C	-3.4003595	1.0111575	4.4145911
H	-3.7124481	1.0134104	5.4700175
C	-2.1147877	0.5676146	4.0704806
H	-1.4356973	0.1983810	4.8537175
C	0.1749392	-1.4802120	3.3794072
C	1.3810284	-1.7086064	4.0705938
H	2.1908006	-0.9659977	4.0171477
C	1.5467909	-2.8765756	4.8343570
H	2.4910630	-3.0423605	5.3749203
C	0.5141474	-3.8239485	4.9138976
H	0.6457181	-4.7362018	5.5150280
C	-0.6911002	-3.6014671	4.2238892
H	-1.5063934	-4.3383801	4.2841612
C	-0.8593206	-2.4397892	3.4576048
H	-1.8055265	-2.2668907	2.9209936
C	1.2271249	1.1425603	2.8477118
C	2.4722378	1.1376377	2.1832450
H	2.6137218	0.5058561	1.2916531
C	3.5071995	1.9709527	2.6309677
H	4.4734933	1.9673439	2.1048509
C	3.2997177	2.8243532	3.7281802
H	4.1085084	3.4875085	4.0708870
C	2.0537996	2.8436865	4.3767978

H	1.8831885	3.5235973	5.2252619
C	1.0176472	2.0020953	3.9415201
H	0.0399501	2.0304748	4.4436323

S3

75

SCF Energy = -4548.330443956

C	-1.9043577	1.2256264	-3.0903848
C	-1.5810157	0.0673859	-2.3385970
C	-2.6373659	-0.6494564	-1.7229744
C	-3.9689503	-0.2307560	-1.8588734
C	-4.2733470	0.9157534	-2.6112212
C	-3.2341025	1.6389591	-3.2258214
C	-0.1838874	-0.3177227	-2.1123481
C	0.8461579	-0.4038035	-2.9904184
C	0.7046896	-0.2682788	-4.4603168
C	-0.3873138	-0.8433298	-5.1520759
C	-0.5165018	-0.6976886	-6.5396462
C	0.4438271	0.0240303	-7.2697546
C	1.5369964	0.5959524	-6.5974416
C	1.6689580	0.4480971	-5.2089451
Br	0.0709195	2.0991488	-0.2577861
C	0.9138929	-2.4852695	-0.9540790
C	-0.1412038	-3.3086821	-1.6575871
C	0.9024064	-2.3861886	0.4441848
C	2.1547868	-2.1618156	-1.7614393
C	2.2148049	-0.7393576	-2.4156458
O	2.6995318	0.2227053	-1.4867682
H	2.9620362	-0.8064679	-3.2347052
H	3.0596808	-2.2548028	-1.1280220
H	2.2377057	-2.9044305	-2.5824273
H	1.8326176	-2.1600271	0.9902926
H	0.1363702	-2.9228725	1.0258024
H	-0.4101387	-2.8789777	-2.6410783
H	-1.0593578	-3.4216802	-1.0507593
H	0.2738417	-4.3240130	-1.8439110
H	1.9553680	0.8235465	-1.2395822
H	-1.1401723	-1.4111506	-4.5861477
H	-1.3727300	-1.1565245	-7.0575634
H	0.3419890	0.1374432	-8.3597001
H	2.2924106	1.1673286	-7.1585833
H	2.5154543	0.9175803	-4.6846809
H	-2.3981747	-1.5383633	-1.1210723
H	-4.7726540	-0.8014473	-1.3689360
H	-5.3169140	1.2498097	-2.7151166
H	-3.4638974	2.5450916	-3.8070216

H	-1.0895255	1.8053570	-3.5448209
Pd	0.1254193	-0.4245225	-0.0756187
P	-0.0320902	-0.0428990	2.2474834
C	-1.7011146	0.5627764	2.7203144
C	-2.6017773	0.9822760	1.7195719
H	-2.2909743	0.9762231	0.6647562
C	-3.8906025	1.4124998	2.0706647
H	-4.5839371	1.7327838	1.2786911
C	-4.2887154	1.4311462	3.4170715
H	-5.2995959	1.7708502	3.6897863
C	-3.3978993	1.0047485	4.4176069
H	-3.7089286	1.0069419	5.4733463
C	-2.1116385	0.5639883	4.0724881
H	-1.4308536	0.1969840	4.8553015
C	1.2276049	1.1459675	2.8462591
C	2.4724462	1.1429901	2.1812673
H	2.6151145	0.5102234	1.2905580
C	3.5056684	1.9793305	2.6273397
H	4.4717214	1.9771990	2.1007758
C	3.2967390	2.8337333	3.7235029
H	4.1040558	3.4994305	4.0647494
C	2.0511545	2.8508878	4.3728169
H	1.8794316	3.5313813	5.2205886
C	1.0167307	2.0063563	3.9391264
H	0.0392386	2.0330842	4.4417313
C	0.1821591	-1.4790646	3.3801309
C	1.3896367	-1.7045603	4.0698776
H	2.1980313	-0.9605948	4.0144676
C	1.5586626	-2.8714861	4.8345065
H	2.5038552	-3.0347868	5.3742156
C	0.5280534	-3.8209041	4.9160922
H	0.6620860	-4.7322235	5.5180949
C	-0.6783765	-3.6015666	4.2271544
H	-1.4919133	-4.3403211	4.2886046
C	-0.8499604	-2.4407792	3.4602671
H	-1.7971782	-2.2702850	2.9246760

S4

75

SCF Energy = -4548.336642912

C	-2.2605826	0.8843552	-1.2414207
C	-1.6418605	-0.0950277	-2.0672399
C	-2.4442814	-1.1512119	-2.5798871
C	-3.8050416	-1.2287984	-2.2655958
C	-4.3961609	-0.2692167	-1.4203177
C	-3.6209909	0.7874500	-0.9167845

C	-0.1909920	-0.1433807	-2.2579625
C	0.6011965	-0.2275525	-3.3451010
C	0.0662031	0.0042941	-4.7108243
C	0.4841086	-0.7825923	-5.8102936
C	-0.0585949	-0.5817631	-7.0882684
C	-1.0248238	0.4155050	-7.2989104
C	-1.4404860	1.2128025	-6.2183745
C	-0.9011287	1.0116276	-4.9414507
Br	1.0070536	2.1550528	-0.4210765
C	1.7750309	-1.9460888	-0.9254791
C	2.9184551	-1.7889685	0.0509717
C	0.5302716	-2.4654273	-0.4997938
C	2.1780120	-1.9438564	-2.3891127
C	2.0760543	-0.5942674	-3.1591844
O	2.8511307	0.4285001	-2.5725370
H	2.5187390	-0.7760926	-4.1613802
H	3.2388720	-2.2668784	-2.4437572
H	1.5731646	-2.6874906	-2.9466581
H	-0.1768364	-2.8534219	-1.2501375
H	0.4294157	-2.8794569	0.5141675
H	3.5022045	-0.8780395	-0.1903384
H	3.6115376	-2.6539380	-0.0508974
H	2.5743146	-1.7466176	1.1020180
H	2.2808292	0.9391091	-1.9444356
H	1.2293851	-1.5785444	-5.6613266
H	0.2756850	-1.2125173	-7.9263845
H	-1.4464972	0.5762148	-8.3026781
H	-2.1854638	2.0081181	-6.3742772
H	-1.2106697	1.6517642	-4.1032664
H	-1.9726898	-1.9048832	-3.2279355
H	-4.4127912	-2.0501225	-2.6756531
H	-5.4624840	-0.3468035	-1.1590525
H	-4.0707577	1.5426454	-0.2554604
H	-1.6506068	1.7153074	-0.8598665
Pd	0.3449514	-0.3145046	-0.3317066
P	0.0213375	-0.2200691	2.0514955
C	1.2054689	0.6991615	3.1051696
C	2.4988999	0.9639296	2.6160616
H	2.7628125	0.6606550	1.5937707
C	3.4260773	1.6451166	3.4208976
H	4.4330521	1.8566660	3.0314042
C	3.0621655	2.0708678	4.7083703
H	3.7879964	2.6112401	5.3349780
C	1.7661392	1.8197455	5.1940426
H	1.4765024	2.1623759	6.1990436
C	0.8370192	1.1386465	4.3946546

H	-0.1817562	0.9502857	4.7667294
C	-0.1904884	-1.8351479	2.8984195
C	0.6122939	-2.2335338	3.9862785
H	1.3574207	-1.5381721	4.3990171
C	0.4612279	-3.5139730	4.5442982
H	1.0949614	-3.8144556	5.3924554
C	-0.4935474	-4.4046993	4.0287955
H	-0.6116975	-5.4053679	4.4709873
C	-1.2928422	-4.0168373	2.9391004
H	-2.0372779	-4.7125054	2.5232541
C	-1.1341003	-2.7463651	2.3674993
H	-1.7414208	-2.4570165	1.4952057
C	-1.5684598	0.6717823	2.3553482
C	-2.7264272	0.0520654	2.8632095
H	-2.7073260	-1.0066122	3.1562287
C	-3.9140155	0.7886440	3.0102208
H	-4.8129559	0.2927123	3.4068680
C	-3.9531859	2.1474908	2.6620547
H	-4.8847717	2.7217609	2.7790748
C	-2.7940449	2.7719840	2.1678836
H	-2.8119441	3.8380127	1.8950286
C	-1.6085467	2.0417910	2.0117779
H	-0.7096181	2.5264912	1.5997594

Optimized Geometries (MXnc)

R3
75
SCF Energy = -4548.341224723

C	2.1698052	2.0847436	0.8564030
C	1.5467395	1.6300254	-0.3318908
C	0.9931745	2.5993737	-1.2068190
C	1.0707130	3.9679159	-0.9140143
C	1.6875007	4.4011962	0.2730445
C	2.2326138	3.4519742	1.1546256
C	1.4192940	0.1961410	-0.6397765
C	2.3797337	-0.7544170	-0.4980258
C	3.7799520	-0.4722013	-0.0884844
C	4.5301131	0.5590085	-0.7027768
C	5.8389821	0.8427384	-0.2934372
C	6.4371711	0.0957818	0.7369816
C	5.7122293	-0.9371418	1.3516289
C	4.3980925	-1.2200692	0.9450924

Br	-2.8882652	-0.4088734	-1.9909818
C	1.1671705	-1.0388299	-3.1817859
C	1.9165700	0.1478836	-3.7311453
C	-0.1857042	-1.1992254	-3.4241793
C	1.9998318	-2.1407124	-2.5605276
C	2.0255092	-2.1568509	-0.9924296
O	2.8400676	-3.2076001	-0.5160548
H	0.9899736	-2.3895789	-0.6599473
H	1.6314347	-3.1347386	-2.8851258
H	3.0516460	-2.0420786	-2.9024838
H	-0.6817262	-2.1663242	-3.2511404
H	-0.7368784	-0.4798097	-4.0474631
H	2.5489077	-0.1895273	-4.5813639
H	2.6000205	0.5803182	-2.9747181
H	1.2369273	0.9403904	-4.0965872
H	3.7713893	-2.9235930	-0.6181966
H	4.0652169	1.1521518	-1.5035694
H	6.3992146	1.6533191	-0.7839578
H	7.4658481	0.3189011	1.0581260
H	6.1688909	-1.5249265	2.1628184
H	3.8273460	-2.0171473	1.4405479
H	0.4791449	2.2593041	-2.1188712
H	0.6343849	4.6994376	-1.6110189
H	1.7380347	5.4742737	0.5121571
H	2.7057354	3.7776979	2.0935320
H	2.5907133	1.3496975	1.5549461
Pd	-0.4284821	-0.3061896	-1.3358947
P	-1.2133637	-0.1141005	0.8017854
C	-2.4440565	1.2243761	0.9958060
C	-2.0383339	2.5360637	0.6703148
H	-1.0151915	2.7257395	0.3143554
C	-2.9479279	3.5964766	0.7836657
H	-2.6242575	4.6172294	0.5301418
C	-4.2668340	3.3534663	1.2045093
H	-4.9825130	4.1857471	1.2845471
C	-4.6738897	2.0445307	1.5097400
H	-5.7103649	1.8472037	1.8225397
C	-3.7670829	0.9780258	1.4061419
H	-4.0926373	-0.0482455	1.6264138
C	-2.0043293	-1.6705632	1.3810652
C	-2.2351042	-2.7453697	0.5019008
H	-1.9875598	-2.6306999	-0.5631277
C	-2.8027108	-3.9357034	0.9836408
H	-2.9781815	-4.7721256	0.2906108
C	-3.1493962	-4.0564635	2.3386690
H	-3.5963819	-4.9901028	2.7128521

C	-2.9207397	-2.9847349	3.2193691
H	-3.1874261	-3.0754063	4.2832322
C	-2.3422205	-1.7982491	2.7466577
H	-2.1437774	-0.9686379	3.4417035
C	-0.0207887	0.1599911	2.1795094
C	-0.0485183	1.2978299	3.0060347
H	-0.8050453	2.0777326	2.8434702
C	0.8945265	1.4427856	4.0380765
H	0.8655805	2.3382265	4.6769530
C	1.8713310	0.4582094	4.2452895
H	2.6144511	0.5757988	5.0483762
C	1.8953326	-0.6861094	3.4264663
H	2.6529805	-1.4658525	3.5914014
C	0.9546819	-0.8374122	2.3999464
H	0.9712453	-1.7383180	1.7697076

R4

75

SCF Energy = -4548.350861461

C	-1.4247687	-2.1041770	-1.8337582
C	-1.5777782	-1.5984382	-0.5190485
C	-2.8440654	-1.0764296	-0.1458515
C	-3.9119949	-1.0557995	-1.0539652
C	-3.7385134	-1.5503103	-2.3584455
C	-2.4919859	-2.0763096	-2.7399680
C	-0.4358065	-1.5299723	0.4081315
C	0.4777548	-2.5019130	0.6538552
C	0.3115448	-3.8888019	0.1435593
C	-0.9158567	-4.5725352	0.3163208
C	-1.1028047	-5.8601077	-0.2024729
C	-0.0628100	-6.5006859	-0.8987279
C	1.1657642	-5.8420757	-1.0673476
C	1.3546298	-4.5502183	-0.5512542
Br	-0.9340286	2.6393441	2.0751221
C	0.3184787	-0.7136784	3.2976155
C	1.2043306	0.3513122	3.9013067
C	-1.0678212	-0.5577726	3.2166791
C	0.9912347	-2.0466394	3.0588586
C	1.6156189	-2.2107665	1.6338271
O	2.6554391	-3.1688857	1.6369325
H	2.0933458	-1.2425853	1.3688751
H	1.8322463	-2.1515453	3.7739879
H	0.2889663	-2.8877613	3.2283050
H	-1.6982613	-1.4365217	3.0095165
H	-1.5564045	0.3294536	3.6461946
H	2.1469694	0.4587344	3.3258866

H	1.4910883	0.0385225	4.9299252
H	0.6997029	1.3339764	3.9431777
H	2.2364294	-4.0535011	1.6356124
H	-1.7293404	-4.0698089	0.8592339
H	-2.0676211	-6.3703435	-0.0600847
H	-0.2095830	-7.5124542	-1.3060721
H	1.9850175	-6.3342645	-1.6137907
H	2.3122327	-4.0326665	-0.6949567
H	-2.9790639	-0.6752381	0.8703294
H	-4.8839657	-0.6448780	-0.7415515
H	-4.5730463	-1.5262812	-3.0755395
H	-2.3441065	-2.4622904	-3.7600304
H	-0.4506045	-2.5084641	-2.1391680
Pd	-0.3842282	0.2822611	1.2606419
P	0.5635140	1.1843313	-0.6436495
C	-0.4960646	2.4512163	-1.4324835
C	0.0083904	3.6925927	-1.8600320
H	1.0681887	3.9398745	-1.7018915
C	-0.8500031	4.6184138	-2.4749572
H	-0.4562880	5.5935656	-2.7994029
C	-2.2050069	4.3052517	-2.6696517
H	-2.8748943	5.0346559	-3.1498436
C	-2.7074100	3.0640289	-2.2410418
H	-3.7700858	2.8162053	-2.3824917
C	-1.8598480	2.1404496	-1.6149456
H	-2.2565211	1.1772122	-1.2608094
C	2.1786392	2.0023010	-0.3118881
C	2.4354552	2.5641517	0.9554101
H	1.6534804	2.5241594	1.7296211
C	3.6610971	3.2004192	1.2040190
H	3.8520468	3.6375893	2.1957401
C	4.6367544	3.2804905	0.1965030
H	5.5992727	3.7753420	0.3970525
C	4.3804588	2.7284016	-1.0697833
H	5.1384416	2.7914968	-1.8652663
C	3.1568647	2.0911050	-1.3266615
H	2.9621999	1.6569885	-2.3179687
C	0.9827862	0.0471512	-2.0266155
C	1.9375059	-0.9676668	-1.7942378
H	2.4430079	-1.0356480	-0.8206651
C	2.2564261	-1.8794829	-2.8089035
H	3.0040017	-2.6640346	-2.6215710
C	1.6232822	-1.7936342	-4.0624938
H	1.8713282	-2.5158410	-4.8548439
C	0.6799373	-0.7827501	-4.2987156
H	0.1820573	-0.7069957	-5.2770433

C	0.3577898	0.1348847	-3.2845559
H	-0.3898545	0.9183074	-3.4711822

S3

75

SCF Energy = -4548.350729778

C	0.5517158	-2.1907089	-2.1012357
C	-0.5861864	-1.6025846	-1.4954572
C	-1.5954488	-1.0755376	-2.3417919
C	-1.4770428	-1.1401646	-3.7371410
C	-0.3358081	-1.7170572	-4.3214206
C	0.6751761	-2.2389737	-3.4955239
C	-0.7175585	-1.4878678	-0.0330986
C	-0.4955833	-2.4614703	0.8883690
C	-0.1420606	-3.8632022	0.5513103
C	-0.7912182	-4.5685651	-0.4889260
C	-0.4224451	-5.8821417	-0.8074847
C	0.6031281	-6.5247323	-0.0921720
C	1.2489666	-5.8429253	0.9524686
C	0.8760938	-4.5295199	1.2742706
Br	-1.9198683	2.8668389	0.4668309
C	-3.0267303	-1.1214279	1.5386408
C	-3.7781766	-1.8650212	0.4630139
C	-3.1948611	0.2434474	1.7030852
C	-2.3020379	-1.9732358	2.5604246
C	-0.7560719	-2.1387548	2.3589526
O	-0.0403191	-1.0201069	2.8548979
H	-0.4436270	-2.9913917	2.9929686
H	-2.4448389	-1.5555855	3.5774969
H	-2.7463831	-2.9896492	2.5450628
H	-2.8648222	0.7470620	2.6244274
H	-3.9026146	0.8032460	1.0743269
H	-4.6157612	-2.4224402	0.9368387
H	-3.1347783	-2.6145822	-0.0371379
H	-4.2035853	-1.1851794	-0.2989130
H	-0.2377045	-0.2767951	2.2186970
H	-1.5924482	-4.0720119	-1.0549051
H	-0.9433357	-6.4115151	-1.6199112
H	0.8927023	-7.5561973	-0.3437833
H	2.0513995	-6.3372924	1.5213874
H	1.3937407	-3.9988732	2.0878038
H	-2.4750140	-0.5953809	-1.8875166
H	-2.2743696	-0.7233443	-4.3707930
H	-0.2335745	-1.7571891	-5.4164319
H	1.5771811	-2.6852132	-3.9410134
H	1.3437590	-2.6036149	-1.4633171

Pd	-1.2718817	0.4076803	0.4846649
P	0.8494983	1.1471259	-0.0123699
C	0.8934531	2.2987244	-1.4304925
C	1.3288806	3.6298846	-1.2957548
H	1.6607353	4.0029454	-0.3166738
C	1.3191901	4.4811802	-2.4117308
H	1.6532405	5.5239688	-2.3020786
C	0.8762015	4.0102015	-3.6584444
H	0.8678338	4.6825672	-4.5297542
C	0.4334933	2.6825259	-3.7890010
H	0.0752453	2.3080258	-4.7597004
C	0.4337703	1.8278002	-2.6783161
H	0.0653831	0.7974211	-2.7797552
C	1.6182877	2.0288658	1.4089565
C	3.0135953	2.2508313	1.3939648
H	3.6170780	1.8996728	0.5439205
C	3.6319945	2.9108573	2.4650204
H	4.7186327	3.0837445	2.4438810
C	2.8680297	3.3403797	3.5641074
H	3.3564919	3.8505008	4.4082980
C	1.4830348	3.1136504	3.5842753
H	0.8793737	3.4461333	4.4419285
C	0.8557896	2.4635544	2.5098266
H	-0.2333541	2.3139505	2.5069235
C	2.1556399	-0.0952920	-0.3810333
C	2.8938501	-0.0919559	-1.5791414
H	2.6974632	0.6701928	-2.3457450
C	3.8770701	-1.0709440	-1.8009792
H	4.4466467	-1.0646070	-2.7424998
C	4.1224898	-2.0562135	-0.8327254
H	4.8841750	-2.8300020	-1.0123523
C	3.3950195	-2.0505419	0.3716507
H	3.5882896	-2.8178987	1.1354157
C	2.4164986	-1.0746073	0.6027795
H	1.8421569	-1.0756361	1.5423825

S4

75

SCF Energy = -4548.359538668

C	-1.1476955	-2.1636887	-1.9407094
C	-1.4922049	-1.6117690	-0.6818748
C	-2.7829647	-1.0388323	-0.5338907
C	-3.6893625	-1.0133554	-1.6033951
C	-3.3249201	-1.5529112	-2.8489824
C	-2.0525703	-2.1293415	-3.0083898
C	-0.5259961	-1.5536943	0.4276317

C	0.2878053	-2.5407604	0.8790704
C	0.2257409	-3.9351968	0.3729999
C	-1.0084041	-4.5973097	0.1765999
C	-1.0507664	-5.8976100	-0.3435471
C	0.1393465	-6.5681464	-0.6757219
C	1.3737804	-5.9291544	-0.4719825
C	1.4168307	-4.6290782	0.0528859
Br	-1.0770956	2.7078758	1.8378953
C	-0.2492883	-0.6372110	3.3930588
C	0.5239904	0.4247343	4.1391601
C	-1.5835070	-0.4477526	3.0267038
C	0.4188312	-1.9953952	3.3246218
C	1.2550100	-2.2576890	2.0293598
O	2.1893874	-1.2155663	1.7844444
H	1.8630155	-3.1644433	2.2153785
H	1.1118042	-2.0757002	4.1871555
H	-0.3277005	-2.8092973	3.4117628
H	-2.1879003	-1.3151660	2.7194745
H	-2.1178208	0.4665562	3.3256028
H	1.5725506	0.4665482	3.7819084
H	0.5667649	0.1403579	5.2142377
H	0.0594712	1.4230706	4.0413978
H	1.6379321	-0.4290789	1.5362768
H	-1.9400080	-4.0758172	0.4389621
H	-2.0220788	-6.3953200	-0.4868250
H	0.1047789	-7.5891725	-1.0849121
H	2.3117515	-6.4465780	-0.7259162
H	2.3872640	-4.1303059	0.1983937
H	-3.0672434	-0.6020541	0.4355374
H	-4.6834318	-0.5624605	-1.4633114
H	-4.0307570	-1.5250299	-3.6928895
H	-1.7548424	-2.5510525	-3.9803199
H	-0.1541162	-2.6107460	-2.0738013
Pd	-0.5269573	0.3030371	1.1967839
P	0.7066257	1.1012253	-0.5970263
C	2.2903602	1.8716749	-0.0653086
C	2.4098092	2.4293929	1.2240592
H	1.5394329	2.4215276	1.8983451
C	3.6194388	3.0182145	1.6224924
H	3.7041475	3.4504193	2.6309051
C	4.7135522	3.0555576	0.7428730
H	5.6627362	3.5131313	1.0608952
C	4.5950717	2.5058297	-0.5448641
H	5.4484494	2.5332247	-1.2392808
C	3.3898083	1.9137239	-0.9504890
H	3.3034126	1.4763423	-1.9556768

C	1.2639717	-0.0909487	-1.8812096
C	0.8554478	0.0148315	-3.2241165
H	0.1967060	0.8373543	-3.5354188
C	1.2796492	-0.9374068	-4.1659476
H	0.9512906	-0.8490560	-5.2124978
C	2.1080676	-1.9991927	-3.7720890
H	2.4318218	-2.7503256	-4.5084066
C	2.5251792	-2.1003365	-2.4322966
H	3.1750018	-2.9304105	-2.1183341
C	2.1080036	-1.1534205	-1.4870051
H	2.4303594	-1.2409276	-0.4379157
C	-0.1982813	2.3812334	-1.5390243
C	0.3789614	3.6237058	-1.8566552
H	1.3996732	3.8580178	-1.5214156
C	-0.3601048	4.5671126	-2.5885191
H	0.0888607	5.5430785	-2.8273678
C	-1.6671558	4.2709595	-3.0074708
H	-2.2436820	5.0143941	-3.5786157
C	-2.2424157	3.0284953	-2.6877567
H	-3.2693726	2.7936722	-3.0054864
C	-1.5159257	2.0864999	-1.9475924
H	-1.9737759	1.1227101	-1.6793661

Optimized Geometries(BXn)(TS-cd)-exo

R1
75
SCF Energy = -4548.297673059

C	1.1481402	4.3305207	-0.6635396
C	0.4251666	3.3075167	0.0158307
C	-0.9705697	3.5115920	0.2623081
C	-1.5912418	4.7199701	-0.1011796
C	-0.8464117	5.7296601	-0.7191947
C	0.5178916	5.5223619	-1.0163055
C	1.0866648	2.1315231	0.5921584
C	1.0592310	0.8030365	0.2940590
C	0.2493802	0.1872407	-0.7718832
C	-0.1729231	-1.1585691	-0.6197152
C	-0.9809289	-1.7710850	-1.5871882
C	-1.3797682	-1.0618857	-2.7327524
C	-0.9581909	0.2693906	-2.9006433
C	-0.1546994	0.8881275	-1.9348612
Br	1.2837990	5.6995095	2.9501429

C	2.8578734	2.2147728	1.8325133
C	3.7825207	3.2571655	1.2414825
C	2.3643782	2.4660521	3.1867079
C	3.1690961	0.7650397	1.4862403
C	1.9139529	-0.0723534	1.1960095
O	1.2304504	-0.5125932	2.3681142
H	2.2215442	-0.9954380	0.6600660
H	3.7988626	0.7526255	0.5728561
H	3.7506373	0.2904071	2.3048499
H	2.1185399	1.5847610	3.8023351
H	2.8148832	3.3095223	3.7369904
H	3.9000758	3.1204083	0.1487926
H	4.7914630	3.1446974	1.6970874
H	3.4242689	4.2847204	1.4536901
H	0.5112915	0.1255770	2.5528859
H	0.1015746	-1.7034895	0.2949317
H	-1.3053141	-2.8132287	-1.4421593
H	-2.0110969	-1.5445031	-3.4939302
H	-1.2536454	0.8312322	-3.7999617
H	0.1792945	1.9237367	-2.0874694
H	-1.5613607	2.6888656	0.6827234
H	-2.6586297	4.8629877	0.1186516
H	-1.3247950	6.6845837	-0.9826648
H	1.0963916	6.3161749	-1.5114320
H	2.2152279	4.1811103	-0.8700753
Pd	0.6802940	3.2752707	2.3357205
P	-1.0787754	2.5042965	3.6767579
C	-2.6320541	3.4343148	3.3456178
C	-2.4977113	4.8272504	3.1526454
H	-1.4941687	5.2882480	3.1687911
C	-3.6372829	5.6119529	2.9239888
H	-3.5256130	6.6969924	2.7772540
C	-4.9099867	5.0169003	2.8690946
H	-5.8011840	5.6345037	2.6795727
C	-5.0428116	3.6307956	3.0574440
H	-6.0373715	3.1605307	3.0192430
C	-3.9088458	2.8391692	3.3025360
H	-4.0190061	1.7556455	3.4576647
C	-1.5199440	0.7380912	3.4713783
C	-1.1278245	-0.2452912	4.4086914
H	-0.6515932	0.0575690	5.3522070
C	-1.3280245	-1.6069543	4.1330519
H	-1.0071952	-2.3598375	4.8684524
C	-1.9256597	-2.0092634	2.9286404
H	-2.0787390	-3.0780438	2.7173722
C	-2.3105170	-1.0409457	1.9855034

H	-2.7603132	-1.3423996	1.0286463
C	-2.0974377	0.3180207	2.2468586
H	-2.3877189	1.0610281	1.4896095
C	-0.8607966	2.7445070	5.4856803
C	0.2188036	3.5298908	5.9342011
H	0.9015882	3.9828640	5.1975027
C	0.3804281	3.7765595	7.3079147
H	1.2212308	4.3974128	7.6521414
C	-0.5303743	3.2434758	8.2332674
H	-0.4004792	3.4363246	9.3091844
C	-1.6196056	2.4736401	7.7850888
H	-2.3442581	2.0683271	8.5076917
C	-1.7905892	2.2299873	6.4153348
H	-2.6521475	1.6415190	6.0644621

R2

75

SCF Energy = -4548.311633101

C	-0.7199096	3.7382082	-1.4534648
C	-1.1980273	2.5729915	-0.7971641
C	-2.4820872	2.0848556	-1.1521503
C	-3.2497687	2.7233080	-2.1364524
C	-2.7557129	3.8636899	-2.7884689
C	-1.4885250	4.3661928	-2.4392204
C	-0.4108740	1.9618269	0.2904126
C	0.9086949	1.6552168	0.3286162
C	1.8421702	1.8454602	-0.8087054
C	1.4836122	1.4742189	-2.1262395
C	2.3813602	1.6462906	-3.1872515
C	3.6592067	2.1864183	-2.9559980
C	4.0334240	2.5472516	-1.6516200
C	3.1358847	2.3754938	-0.5860803
Br	-0.4322019	4.8797047	1.8128829
C	-1.0258372	0.3680466	1.6339295
C	-1.0792095	-0.7083479	0.5645778
C	-2.2521233	0.7227948	2.3032864
C	0.2754822	0.4494608	2.4202988
C	1.4510519	0.8932282	1.5319362
O	2.1319801	-0.2891151	1.0909604
H	2.1457052	1.5343891	2.1280838
H	0.1495755	1.1500047	3.2681003
H	0.5330075	-0.5499494	2.8320935
H	-2.2542738	0.7516069	3.4070905
H	-3.1983222	0.3592708	1.8679224
H	-1.2732980	-1.6758750	1.0787250
H	-0.1185848	-0.7935895	0.0262174

H	-1.8993863	-0.5473527	-0.1588640
H	2.7156396	-0.0174210	0.3536664
H	0.4886675	1.0428097	-2.3065267
H	2.0840010	1.3505667	-4.2049266
H	4.3630591	2.3207616	-3.7911585
H	5.0303107	2.9729301	-1.4606355
H	3.4255542	2.6837392	0.4299606
H	-2.8850110	1.2013014	-0.6389028
H	-4.2463235	2.3303347	-2.3877045
H	-3.3601897	4.3671360	-3.5578476
H	-1.0984578	5.2696864	-2.9322786
H	0.2465728	4.1587286	-1.1476818
Pd	-1.7087166	2.6851725	1.8225767
P	-3.4807168	3.6899902	2.8325284
C	-3.1275862	4.8318577	4.2211404
C	-4.4496876	4.6482072	1.5974799
C	-4.7295912	2.5363915	3.5364040
C	-3.9959943	5.8887373	4.5552161
C	-3.7156056	6.6983861	5.6670382
C	-2.5726949	6.4539456	6.4472782
C	-1.7023918	5.4033702	6.1102501
C	-1.9728124	4.5979246	4.9941618
H	-4.8855087	6.0869137	3.9391234
H	-4.3914434	7.5288036	5.9217752
H	-2.3535080	7.0928795	7.3162993
H	-0.7972196	5.2210829	6.7086811
H	-1.2804187	3.7966352	4.6953097
C	-5.8407599	4.8410192	1.7496787
C	-6.5567872	5.5775834	0.7937999
C	-5.8921228	6.1230858	-0.3180128
C	-4.5096792	5.9299915	-0.4709105
C	-3.7856915	5.1947373	0.4795650
H	-6.3675849	4.4021595	2.6101060
H	-7.6408102	5.7230635	0.9174754
H	-6.4566789	6.6967454	-1.0690383
H	-3.9821126	6.3459030	-1.3415777
H	-2.7000790	5.0492648	0.3648285
C	-4.9124533	2.3917941	4.9250998
C	-5.8100257	1.4308625	5.4220572
C	-6.5332270	0.6140738	4.5392818
C	-6.3543004	0.7561140	3.1510188
C	-5.4529596	1.7055459	2.6517300
H	-4.3550517	3.0375424	5.6195994
H	-5.9473998	1.3264478	6.5090657
H	-7.2385993	-0.1344367	4.9306794
H	-6.9205569	0.1203339	2.4534285

H	-5.3116360	1.8162397	1.5649901
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R3

75

SCF Energy = -4548.313087721

C	-0.9987642	5.7904963	0.0635466
C	-0.7042357	4.4046010	0.0561261
C	-1.0433257	3.6621636	-1.1056013
C	-1.6219263	4.2861211	-2.2167281
C	-1.8958721	5.6656547	-2.1949606
C	-1.5856184	6.4126022	-1.0467293
C	-0.1428281	3.7242297	1.2303699
C	0.6533425	2.6205327	1.2604702
C	1.4632284	2.1513940	0.1184350
C	1.5197129	0.7845110	-0.2545417
C	2.2867745	0.3819520	-1.3592297
C	3.0141987	1.3275512	-2.1004669
C	2.9728699	2.6838696	-1.7298490
C	2.2070170	3.0954074	-0.6328766
Br	2.1861486	5.8392148	1.9490610
C	-1.5161564	3.1113584	2.7901967
C	-2.6824886	2.9125206	1.8452466
C	-1.6642330	4.1362754	3.7956298
C	-0.7049107	1.8658788	3.1583860
C	0.7385097	1.9365377	2.6377708
O	1.2671985	0.6236889	2.6441605
H	1.3518355	2.6031886	3.2975224
H	-0.7137202	1.7053246	4.2553915
H	-1.1632963	0.9751065	2.6815218
H	-1.3706842	3.8953556	4.8321607
H	-2.5521480	4.7884137	3.7278683
H	-2.4203730	2.2760813	0.9800740
H	-3.0676901	3.8771181	1.4633339
H	-3.5005825	2.4148095	2.4120832
H	2.1748854	0.6731557	2.2873223
H	0.9374908	0.0470464	0.3142098
H	2.3093393	-0.6805076	-1.6470665
H	3.6150400	1.0078186	-2.9656423
H	3.5485195	3.4292821	-2.2996436
H	2.1863417	4.1497297	-0.3160938
H	-0.8399905	2.5821589	-1.1281824
H	-1.8674928	3.6886902	-3.1081476
H	-2.3545501	6.1536261	-3.0684459
H	-1.7970810	7.4922594	-1.0136709
H	-0.7461468	6.3791420	0.9586078
Pd	-0.0096678	5.0453209	2.9405002

P	0.1342279	6.6806500	4.5373088
C	-0.1684021	8.3912103	3.9275234
C	0.2224430	8.7306286	2.6150019
H	0.7117606	7.9708409	1.9836124
C	0.0222303	10.0358544	2.1403139
H	0.3321448	10.2912593	1.1156881
C	-0.5666604	11.0092807	2.9643240
H	-0.7255223	12.0309608	2.5867773
C	-0.9516935	10.6760814	4.2736940
H	-1.4102534	11.4347882	4.9260501
C	-0.7547004	9.3728783	4.7565301
H	-1.0650128	9.1167928	5.7801394
C	1.7457425	6.7455443	5.4104981
C	2.5065900	5.5622487	5.4934804
H	2.1539002	4.6600750	4.9709611
C	3.7110690	5.5521032	6.2117693
H	4.3041115	4.6271320	6.2703668
C	4.1685078	6.7257807	6.8345572
H	5.1199869	6.7203150	7.3878135
C	3.4180296	7.9099517	6.7402258
H	3.7803800	8.8331839	7.2172560
C	2.2066293	7.9222324	6.0313456
H	1.6238664	8.8518682	5.9512383
C	-1.0788329	6.5075295	5.9113393
C	-0.6913700	6.0452515	7.1844043
H	0.3720096	5.8644740	7.3995904
C	-1.6584891	5.8213241	8.1790728
H	-1.3444126	5.4623579	9.1709550
C	-3.0159354	6.0603236	7.9137918
H	-3.7709804	5.8874289	8.6954232
C	-3.4077644	6.5226957	6.6447497
H	-4.4701098	6.7140053	6.4300258
C	-2.4474234	6.7383311	5.6470091
H	-2.7582286	7.1007640	4.6546953

R4

75

SCF Energy = -4548.284203803

C	2.6019619	0.3405809	-0.3584184
C	1.3101758	0.9148291	-0.2866735
C	0.3272207	0.4770310	-1.2042113
C	0.6347871	-0.4841385	-2.1776795
C	1.9273965	-1.0285059	-2.2542717
C	2.9084366	-0.6141464	-1.3376779
C	1.0283693	1.9289890	0.7634953
Pd	-0.2915538	5.2743771	0.8422542

P	-1.6514391	7.0348029	0.6500834
C	0.3274467	3.0682886	0.5551348
Br	1.6937953	6.3400143	-0.3800974
C	-0.4145827	3.4011640	-0.6840351
C	0.2545862	3.6728769	-1.9058343
C	-0.4773519	3.8959783	-3.0747639
C	-1.8847264	3.8757746	-3.0567365
C	-2.5623147	3.6011095	-1.8594967
C	-1.8374173	3.3492552	-0.6849400
C	1.3844868	1.5779711	2.2088124
O	1.4975010	0.1915491	2.4592858
C	0.2464146	2.2550082	2.9913021
C	0.1715845	3.7103298	2.5587635
C	-1.0906972	4.4460942	2.5810051
C	1.4168260	4.4828527	3.0131060
H	2.3625872	2.0099737	2.5143868
H	0.4272990	2.2146916	4.0877113
H	-0.7003048	1.7206070	2.7718667
H	-2.0178032	3.8539150	2.4847024
H	-1.1813183	5.2828999	3.2962182
H	1.6927844	4.1715657	4.0449179
H	1.2469724	5.5758578	3.0038089
H	2.2860745	4.2958662	2.3549484
H	0.8226321	-0.2595037	1.9149774
H	-0.6880814	0.8924220	-1.1502643
H	-0.1452151	-0.8103951	-2.8823296
H	2.1683884	-1.7794677	-3.0218842
H	3.9226001	-1.0392994	-1.3842901
H	3.3728866	0.6549701	0.3594504
H	-2.3597186	3.0827063	0.2452494
H	-3.6620962	3.5795593	-1.8384472
H	-2.4525600	4.0817604	-3.9755129
H	0.0571708	4.1090863	-4.0126374
H	1.3504708	3.7294790	-1.9058195
C	-2.3145493	7.1310832	-1.0624806
C	-0.9434658	8.6921285	0.9624729
C	-3.1416803	6.9640570	1.7218724
C	-3.4447989	7.9656783	2.6638138
C	-4.5641238	7.8270866	3.5030031
C	-5.3902523	6.6974670	3.4011450
C	-5.0908439	5.6946336	2.4605456
C	-3.9675342	5.8207918	1.6334774
H	-2.8039858	8.8561057	2.7413221
H	-4.7911786	8.6125728	4.2397131
H	-6.2676279	6.5936193	4.0572084
H	-5.7338865	4.8052285	2.3777603

H	-3.7188869	5.0313942	0.9078644
C	-3.6935979	7.2235284	-1.3400964
C	-4.1361582	7.3007806	-2.6709089
C	-3.2084286	7.3004729	-3.7249818
C	-1.8342449	7.2132341	-3.4454737
C	-1.3828376	7.1182779	-2.1221344
H	-4.4247148	7.2405290	-0.5193147
H	-5.2142868	7.3698226	-2.8818921
H	-3.5582352	7.3651572	-4.7667225
H	-1.1017392	7.2026798	-4.2665085
H	-0.3066244	7.0168659	-1.8991631
C	0.2108796	8.8035273	1.7604420
C	0.7399640	10.0706028	2.0493568
C	0.1264470	11.2240330	1.5329454
C	-1.0181135	11.1125810	0.7239500
C	-1.5541161	9.8484893	0.4357806
H	0.7026311	7.8883738	2.1211503
H	1.6471879	10.1552773	2.6660194
H	0.5489443	12.2165207	1.7520390
H	-1.4919247	12.0152049	0.3092208
H	-2.4439392	9.7556651	-0.2054740

S1

75

SCF Energy = -4548.284551216

C	-0.2754617	3.8087611	0.2795252
C	-0.3895729	2.4223774	0.5636926
C	-1.6889171	1.8391492	0.6016548
C	-2.8324708	2.6278290	0.4022081
C	-2.7009979	3.9980673	0.1330018
C	-1.4203122	4.5781094	0.0594747
C	0.8030429	1.5558610	0.7092639
C	1.6187048	1.1905100	-0.3102612
C	1.5711164	1.7454333	-1.6888378
C	0.3639593	2.0198661	-2.3721318
C	0.3848732	2.5304328	-3.6774795
C	1.6060193	2.7808106	-4.3258703
C	2.8113352	2.4984856	-3.6622689
C	2.7959995	1.9782435	-2.3602556
Br	1.2497819	4.2038124	3.2635496
C	1.4069376	0.1609985	2.1674803
C	2.5651172	0.6552800	3.0552783
C	0.1488004	-0.1094442	2.8681997
C	1.8964353	-0.7529396	1.0532228
C	2.6101119	0.0759270	-0.0276622
O	3.9175121	0.5361431	0.3189109

H	2.7589228	-0.5402628	-0.9381950
H	2.5804926	-1.5139785	1.4864619
H	1.0432497	-1.2803365	0.5821674
H	-0.6281307	-0.6565460	2.3048729
H	0.2116775	-0.4156283	3.9274866
H	2.9436817	1.6522828	2.7528706
H	3.4112853	-0.0618744	3.0268634
H	2.2321173	0.7767578	4.1043711
H	3.8008652	1.2991645	0.9171317
H	-0.5985006	1.8180789	-1.8842462
H	-0.5657762	2.7321461	-4.1944223
H	1.6175500	3.1882378	-5.3482584
H	3.7744060	2.6841327	-4.1621174
H	3.7375355	1.7562330	-1.8358929
H	-1.7797582	0.7542693	0.7548115
H	-3.8301531	2.1673974	0.4553145
H	-3.5973425	4.6174463	-0.0149057
H	-1.3147073	5.6520837	-0.1548893
H	0.7228690	4.2636604	0.2607078
Pd	0.0358273	1.9697217	2.8749046
P	-1.4826288	2.2233160	4.4851372
C	-2.7794410	3.3996510	3.9255701
C	-2.3524469	4.6581341	3.4505631
H	-1.2734030	4.8843247	3.4016288
C	-3.3006530	5.5980876	3.0248680
H	-2.9605459	6.5773078	2.6557937
C	-4.6710454	5.2883637	3.0488231
H	-5.4112008	6.0267418	2.7043025
C	-5.0946160	4.0314071	3.5096533
H	-6.1665174	3.7821566	3.5321112
C	-4.1538096	3.0880313	3.9545839
H	-4.4932091	2.1114974	4.3284384
C	-2.3961227	0.6915816	4.9232186
C	-2.4319007	0.1796498	6.2344093
H	-1.9383861	0.7281804	7.0498138
C	-3.0968932	-1.0302815	6.4993664
H	-3.1163466	-1.4257908	7.5262054
C	-3.7354751	-1.7290737	5.4635392
H	-4.2578099	-2.6743100	5.6748309
C	-3.7015332	-1.2206746	4.1518426
H	-4.1978926	-1.7661597	3.3349153
C	-3.0267200	-0.0237079	3.8803417
H	-2.9813104	0.3693996	2.8533582
C	-0.9099860	2.8918974	6.0876606
C	0.4475694	2.7630308	6.4372346
H	1.1487489	2.3290366	5.7095608

C	0.8937986	3.2272082	7.6839642
H	1.9567227	3.1338050	7.9521564
C	-0.0094796	3.8298883	8.5751871
H	0.3444347	4.2022859	9.5486149
C	-1.3625385	3.9725048	8.2202419
H	-2.0678495	4.4558299	8.9131471
C	-1.8152273	3.5064152	6.9768489
H	-2.8713936	3.6248553	6.6902717

S2

75

SCF Energy = -4548.322221800

C	-0.4125416	4.1757735	-1.0191032
C	-0.7782921	3.2239259	-0.0289050
C	-2.1553910	3.0911576	0.2886602
C	-3.1271217	3.8598016	-0.3675394
C	-2.7493153	4.7842094	-1.3535617
C	-1.3870809	4.9372599	-1.6722351
C	0.2705220	2.5325390	0.7368223
C	1.4709826	2.0203727	0.3657281
C	1.9769655	1.9271631	-1.0173248
C	1.1407643	1.5384937	-2.0899717
C	1.6473974	1.4556727	-3.3934047
C	2.9957830	1.7613061	-3.6507243
C	3.8358254	2.1443218	-2.5912344
C	3.3353307	2.2228444	-1.2838301
Br	1.4401325	5.4679371	1.6387899
C	-0.0305366	1.1912599	2.4187282
C	-0.7987835	0.1663745	1.6001842
C	-0.7376620	1.8707271	3.4781879
C	1.4496097	0.8880341	2.5966188
C	2.3639815	1.5507137	1.5090825
O	3.1594388	2.6099174	2.0149725
H	3.0814030	0.7907777	1.1354175
H	1.8062883	1.2325967	3.5859913
H	1.5872635	-0.2135129	2.5573375
H	-0.2647666	1.9141440	4.4744622
H	-1.8367320	1.7751012	3.5121049
H	-0.9144733	-0.7431588	2.2310310
H	-0.2596196	-0.1154568	0.6764421
H	-1.8129997	0.5079752	1.3250510
H	2.6399843	3.4540536	1.9401036
H	0.0870047	1.2949828	-1.8892860
H	0.9855236	1.1457652	-4.2166205
H	3.3910498	1.6984881	-4.6759756
H	4.8913591	2.3892820	-2.7852349

H	3.9774171	2.5461088	-0.4505776
H	-2.4653311	2.3904170	1.0749266
H	-4.1867084	3.7424222	-0.0953916
H	-3.5112407	5.3911443	-1.8655401
H	-1.0769892	5.6719715	-2.4307174
H	0.6513867	4.3314122	-1.2376180
Pd	-0.0626311	3.6096206	2.5510336
P	-0.8912125	5.0478187	4.1114268
C	-2.1059480	6.1928854	3.3439381
C	-2.0368882	6.4433730	1.9575408
H	-1.2496692	5.9670383	1.3537663
C	-2.9669947	7.3044880	1.3559784
H	-2.9067922	7.4852890	0.2728238
C	-3.9669470	7.9189633	2.1268681
H	-4.6965508	8.5917576	1.6506727
C	-4.0410238	7.6685246	3.5081974
H	-4.8266075	8.1432948	4.1155750
C	-3.1172054	6.8057158	4.1169269
H	-3.1925839	6.5930904	5.1940075
C	-1.8593046	4.2654842	5.4653121
C	-1.3600922	4.1707488	6.7786799
H	-0.4014524	4.6458032	7.0345246
C	-2.0883459	3.4778882	7.7611123
H	-1.6917320	3.4114778	8.7856129
C	-3.3172249	2.8799630	7.4415000
H	-3.8872140	2.3413434	8.2134787
C	-3.8192794	2.9726830	6.1306297
H	-4.7838481	2.5084344	5.8746448
C	-3.0927425	3.6553592	5.1458878
H	-3.4863919	3.7287764	4.1197670
C	0.3452072	6.0674211	4.9966048
C	1.6261831	5.5125944	5.1943244
H	1.8630729	4.5315939	4.7541923
C	2.5928800	6.2239560	5.9193930
H	3.5928763	5.7894707	6.0667689
C	2.2910324	7.4969448	6.4325029
H	3.0544115	8.0605087	6.9902063
C	1.0201586	8.0575434	6.2210582
H	0.7870005	9.0603254	6.6100458
C	0.0448944	7.3447728	5.5058779
H	-0.9455667	7.7899506	5.3311355

S3

75

SCF Energy = -4548.322188901

C	-0.0415537	5.2239124	-0.5573673
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C	-0.6061273	4.4105619	0.4623278
C	-1.9512970	4.6586819	0.8416232
C	-2.7067807	5.6609072	0.2168230
C	-2.1378025	6.4447690	-0.7986806
C	-0.8014565	6.2201739	-1.1787481
C	0.2493719	3.4629526	1.1933264
C	1.2502806	2.6450076	0.7805102
C	1.6528273	2.4153688	-0.6204690
C	0.6978948	2.2649502	-1.6530535
C	1.1073344	2.0458864	-2.9747373
C	2.4759308	1.9754698	-3.2906628
C	3.4325470	2.1193786	-2.2713130
C	3.0279406	2.3325668	-0.9458416
Br	2.2023803	5.9789268	2.0018049
C	-0.3299173	2.2563865	2.9047595
C	-1.3848433	1.4797166	2.1340348
C	-0.7759458	3.1038119	3.9850144
C	1.0179360	1.5604872	3.0221369
C	2.0316106	1.9548580	1.8933286
O	3.1001458	2.7637015	2.3564346
H	2.5047948	1.0306223	1.5010277
H	1.4960394	1.7893283	3.9935848
H	0.8485936	0.4633675	2.9833740
H	-0.2639197	3.0178023	4.9590287
H	-1.8569011	3.3107061	4.0691071
H	-0.9858535	1.0623389	1.1907956
H	-2.2795660	2.0845467	1.9005868
H	-1.7142177	0.6356166	2.7803844
H	2.8243773	3.7161236	2.2873243
H	-0.3729468	2.3158206	-1.4067041
H	0.3518755	1.9248868	-3.7662297
H	2.7953998	1.8062359	-4.3301793
H	4.5057714	2.0698427	-2.5111078
H	3.7684285	2.4720350	-0.1438072
H	-2.4031296	4.0714286	1.6517300
H	-3.7445505	5.8372244	0.5369705
H	-2.7286229	7.2349247	-1.2861247
H	-0.3386515	6.8408572	-1.9609984
H	1.0133642	5.0837769	-0.8245877
Pd	0.3003340	4.5934172	3.0052678
P	-0.0351480	6.2025485	4.5823252
C	-0.9304299	7.6335137	3.8570211
C	-0.8655482	7.8541757	2.4653566
H	-0.2676032	7.1817813	1.8318775
C	-1.5569701	8.9343508	1.8963550
H	-1.5044863	9.0907756	0.8089647

C	-2.3134880	9.7977343	2.7050619
H	-2.8566906	10.6424614	2.2544138
C	-2.3834437	9.5783656	4.0918984
H	-2.9801226	10.2487359	4.7290914
C	-1.6983199	8.4982042	4.6683331
H	-1.7748388	8.3147298	5.7506631
C	1.4715188	6.8481805	5.3974853
C	2.5605675	5.9651873	5.5465053
H	2.5007530	4.9560881	5.1102575
C	3.7170538	6.3871203	6.2179302
H	4.5665929	5.6965858	6.3273148
C	3.7976957	7.6951849	6.7253161
H	4.7107920	8.0300741	7.2405815
C	2.7193590	8.5809559	6.5618742
H	2.7865935	9.6100339	6.9461916
C	1.5547020	8.1599843	5.9007324
H	0.7160562	8.8582862	5.7634194
C	-1.1136633	5.7107181	5.9887823
C	-0.5975355	5.4861016	7.2797060
H	0.4643229	5.6858255	7.4861307
C	-1.4385781	5.0153843	8.3027753
H	-1.0270499	4.8454807	9.3093097
C	-2.7964531	4.7697982	8.0464645
H	-3.4533845	4.4047021	8.8502615
C	-3.3158238	4.9933981	6.7583465
H	-4.3804387	4.8053803	6.5518261
C	-2.4793773	5.4549522	5.7331874
H	-2.8863195	5.6309702	4.7248660

S4

75

SCF Energy = -4548.281567865

C	-0.8428647	4.3691572	-0.5995209
C	-0.7310152	3.3730844	0.4043931
C	-1.8828347	2.5922917	0.7046144
C	-3.1055760	2.8388239	0.0686106
C	-3.2055576	3.8511031	-0.9021775
C	-2.0659208	4.5946591	-1.2449658
C	0.5281970	3.0292956	1.1293699
C	1.3943162	2.0636703	0.7277429
C	1.4744902	1.6128000	-0.6809582
C	1.3712109	0.2451254	-1.0238125
C	1.4216333	-0.1620171	-2.3641559
C	1.5906131	0.7888140	-3.3855731
C	1.7121789	2.1487712	-3.0566160
C	1.6549444	2.5577274	-1.7167268

Br	1.2255291	6.5715024	1.0581365
C	0.8947826	3.0040354	3.1764523
C	2.0676515	3.9129636	3.5895788
C	-0.4099595	3.3784076	3.7313550
C	1.3315201	1.5483517	3.0674316
C	2.2003980	1.3635564	1.8064942
O	3.5476899	1.8086236	1.9153177
H	2.2810577	0.2818887	1.5684616
H	1.8937809	1.2641888	3.9828035
H	0.4459415	0.8867896	2.9833284
H	-1.2322560	2.6505059	3.6242629
H	-0.4190402	3.9019180	4.7037206
H	2.6277217	4.3062804	2.7183263
H	2.7771745	3.3559976	4.2364119
H	1.7090910	4.8072014	4.1353651
H	3.5394674	2.7779193	1.8060517
H	1.2254485	-0.5057983	-0.2322557
H	1.3259888	-1.2296022	-2.6143982
H	1.6344639	0.4674932	-4.4372969
H	1.8591685	2.8981223	-3.8491495
H	1.7787346	3.6168776	-1.4501437
H	-1.7987493	1.7897793	1.4521916
H	-3.9866528	2.2319453	0.3281941
H	-4.1678997	4.0560862	-1.3935449
H	-2.1318508	5.3804781	-2.0105198
H	0.0287279	4.9986651	-0.8210212
Pd	-0.2648956	4.8558194	2.2666860
P	-1.9026965	6.2004360	2.9594274
C	-1.4195389	7.7766698	3.7516825
C	-0.1018877	7.9307711	4.2219600
H	0.6237839	7.1209033	4.0538645
C	0.2792645	9.1260758	4.8516616
H	1.3122477	9.2482714	5.2101139
C	-0.6493971	10.1685379	5.0036754
H	-0.3467357	11.1080066	5.4908251
C	-1.9620319	10.0214694	4.5200375
H	-2.6856016	10.8438574	4.6267907
C	-2.3485375	8.8293513	3.8906195
H	-3.3703392	8.7152547	3.4969145
C	-3.0834044	5.4100535	4.1208215
C	-3.3898433	5.9479390	5.3851714
H	-2.9436567	6.9031231	5.6980852
C	-4.2629246	5.2621010	6.2475731
H	-4.4933586	5.6858802	7.2368211
C	-4.8398397	4.0459230	5.8508627
H	-5.5253719	3.5134946	6.5273421

C	-4.5336144	3.5051257	4.5884595
H	-4.9791288	2.5490295	4.2740881
C	-3.6510507	4.1753882	3.7314436
H	-3.3901202	3.7454838	2.7513889
C	-2.9291944	6.7246836	1.5264363
C	-4.3022464	6.4333528	1.4153050
H	-4.8190405	5.8831856	2.2140472
C	-5.0168437	6.8512564	0.2799963
H	-6.0889474	6.6165464	0.1966661
C	-4.3699180	7.5687001	-0.7379403
H	-4.9333564	7.8970230	-1.6247031
C	-2.9998236	7.8635595	-0.6228031
H	-2.4843272	8.4202756	-1.4200885
C	-2.2752436	7.4369112	0.4975356
H	-1.1905235	7.6252801	0.5694014

Optimized Geometries(MXn)(TS-cd)-exo

R3
75
SCF Energy = -4548.313313657

C	1.9560263	4.8470913	-3.0484575
C	1.9136423	4.6605127	-1.6413528
C	1.2745904	5.6681780	-0.8689127
C	0.6921652	6.7903754	-1.4732969
C	0.7395526	6.9514054	-2.8681773
C	1.3783449	5.9724302	-3.6474440
C	2.6337123	3.5297997	-1.0144175
C	2.8884782	2.2816726	-1.5362747
C	2.2450989	1.6645614	-2.7085351
C	0.8910538	1.9486020	-3.0256408
C	0.2638986	1.3461426	-4.1210574
C	0.9667109	0.4319999	-4.9273255
C	2.2984947	0.1183532	-4.6133968
C	2.9305520	0.7199907	-3.5155853
Br	5.2648850	6.3006314	1.5694388
C	2.4321704	3.0425908	0.8544496
C	0.9164726	2.8447598	0.8715520
C	2.9610645	4.0674773	1.7411817
C	3.2174419	1.7205806	0.8212600
C	3.7644527	1.4247866	-0.6035855
O	3.8278395	0.0427588	-0.8936480
H	4.8161815	1.7758860	-0.6754357

H	4.0380089	1.7288349	1.5629308
H	2.5398939	0.8842793	1.0945492
H	3.7461785	3.7836557	2.4598189
H	2.2794848	4.8537115	2.1083015
H	0.6477271	2.3887117	1.8491407
H	0.5896953	2.1615501	0.0634447
H	0.3554312	3.7914439	0.7774619
H	2.9127486	-0.2728474	-1.0307788
H	0.3299423	2.6535344	-2.3967448
H	-0.7866450	1.5861417	-4.3446367
H	0.4727183	-0.0415396	-5.7891019
H	2.8550314	-0.6039909	-5.2300458
H	3.9663927	0.4566732	-3.2680652
H	1.2560898	5.5886694	0.2248894
H	0.2114544	7.5528731	-0.8423387
H	0.2920788	7.8375644	-3.3424393
H	1.4444461	6.0882593	-4.7395059
H	2.4633878	4.1045290	-3.6748052
Pd	4.0727242	4.7007485	0.0923605
P	5.4820956	5.3120458	-1.6677866
C	5.5426138	7.1382788	-1.8233179
C	4.3097561	7.8226182	-1.7695844
H	3.3785874	7.2612362	-1.6022284
C	4.2753465	9.2154460	-1.9180441
H	3.3098342	9.7418056	-1.8778330
C	5.4698772	9.9349992	-2.0978126
H	5.4436550	11.0305498	-2.2008260
C	6.6983259	9.2553672	-2.1329874
H	7.6363756	9.8169770	-2.2601158
C	6.7377799	7.8575045	-2.0000578
H	7.7007829	7.3268936	-2.0212713
C	7.2267324	4.7551910	-1.4862422
C	7.7070152	4.3717060	-0.2174765
H	7.0359076	4.4350424	0.6529759
C	9.0362883	3.9451250	-0.0703180
H	9.4036299	3.6485130	0.9237818
C	9.8925871	3.8969359	-1.1825705
H	10.9334885	3.5590010	-1.0640566
C	9.4175387	4.2787178	-2.4490566
H	10.0840585	4.2419030	-3.3242671
C	8.0895996	4.7045240	-2.6032574
H	7.7166849	4.9920306	-3.5977024
C	5.1091777	4.7747198	-3.3867138
C	4.7429049	5.6817305	-4.4011196
H	4.7097413	6.7583868	-4.1840189
C	4.4055621	5.2124674	-5.6803332

H	4.1165096	5.9293451	-6.4639586
C	4.4354206	3.8366090	-5.9587277
H	4.1666979	3.4673529	-6.9598182
C	4.8188913	2.9299870	-4.9554249
H	4.8546884	1.8541666	-5.1741014
C	5.1474921	3.3934551	-3.6739541
H	5.4499859	2.6817228	-2.8908756

R4

75

SCF Energy = -4548.282843287

C	1.8205174	4.4978894	-2.5680283
C	1.4659191	4.2309770	-1.2180802
C	0.5799682	5.1370643	-0.5679475
C	0.1257583	6.2905561	-1.2268347
C	0.5205670	6.5579744	-2.5477678
C	1.3596834	5.6478062	-3.2155039
C	1.9043989	2.9766310	-0.5483933
C	1.6507279	1.7368516	-1.0473712
C	1.0399983	1.4625330	-2.3733374
C	-0.1198746	2.1326514	-2.8252627
C	-0.6630791	1.8488910	-4.0862513
C	-0.0626461	0.8883559	-4.9173034
C	1.0737349	0.1952693	-4.4676480
C	1.6132144	0.4719805	-3.2039135
Br	3.5018858	6.5442910	2.1395823
C	2.4126236	2.4745985	1.3463739
C	3.8838469	2.0328791	1.4829407
C	2.0395375	3.6254024	2.1669916
C	1.5114191	1.2435252	1.2692414
C	1.7869882	0.5600953	-0.0808042
O	0.9298526	-0.5264618	-0.3644669
H	2.8106073	0.1249497	-0.0842986
H	1.7315668	0.5765304	2.1304709
H	0.4405643	1.5292090	1.3093398
H	0.9632511	3.8470623	2.2713120
H	2.6312059	3.8343965	3.0732453
H	4.2889107	1.6264820	0.5372179
H	3.9532256	1.2256989	2.2452298
H	4.5463927	2.8635298	1.7929534
H	0.0762429	-0.1557975	-0.6636707
H	-0.5949170	2.8850014	-2.1805008
H	-1.5646236	2.3836213	-4.4215622
H	-0.4877012	0.6704577	-5.9087462
H	1.5404241	-0.5721616	-5.1038632
H	2.4919733	-0.0847223	-2.8482790

H	0.2331605	4.9228411	0.4512423
H	-0.5436777	6.9838679	-0.6962767
H	0.1685880	7.4663782	-3.0590089
H	1.6616519	5.8331398	-4.2571004
H	2.4467125	3.7787466	-3.1063587
Pd	3.0956720	4.6209136	0.6531042
P	4.8445097	5.1995442	-0.8101368
C	4.9194239	6.9605097	-1.3017150
C	6.1258156	7.5968462	-1.6540900
H	7.0761345	7.0450354	-1.5923153
C	6.1109344	8.9353135	-2.0767320
H	7.0541388	9.4339770	-2.3473159
C	4.8953851	9.6379572	-2.1490832
H	4.8873719	10.6883463	-2.4782563
C	3.6937434	9.0045905	-1.7892871
H	2.7417894	9.5548051	-1.8315477
C	3.7036212	7.6706666	-1.3565824
H	2.7714629	7.1748434	-1.0498604
C	6.5016776	4.8298687	-0.0930610
C	6.7156628	5.0778636	1.2802794
H	5.8937822	5.4891079	1.8897712
C	7.9683453	4.8131417	1.8534165
H	8.1265114	5.0116070	2.9244305
C	9.0136452	4.2952312	1.0694150
H	9.9934171	4.0835744	1.5242767
C	8.8040868	4.0474899	-0.2970452
H	9.6187775	3.6436637	-0.9174863
C	7.5542121	4.3139785	-0.8791295
H	7.3940969	4.1163077	-1.9492156
C	4.8967061	4.2963107	-2.4085009
C	4.8336384	2.8859890	-2.3656296
H	4.8479798	2.3713881	-1.3935807
C	4.7252073	2.1457956	-3.5496240
H	4.6704875	1.0485803	-3.5066547
C	4.6659055	2.8062414	-4.7902402
H	4.5558045	2.2252662	-5.7179892
C	4.7463867	4.2073856	-4.8393548
H	4.7069473	4.7280567	-5.8082177
C	4.8665081	4.9522949	-3.6542590
H	4.9086541	6.0502230	-3.6925430

S3

75

SCF Energy = -4548.327666277

C	1.2452779	3.7580659	-2.7840760
C	0.6138933	4.0113530	-1.5375150

C	-0.6669736	4.6278830	-1.5686304
C	-1.2929841	4.9480909	-2.7806860
C	-0.6538702	4.6798004	-4.0025083
C	0.6201213	4.0878002	-3.9920960
C	1.3309315	3.7718988	-0.2672873
C	2.3183298	2.8593197	0.0309915
C	2.7488931	1.6807920	-0.7348061
C	1.8575710	0.9714223	-1.5788169
C	2.2746230	-0.1761753	-2.2624618
C	3.5907852	-0.6514176	-2.1196998
C	4.4805839	0.0259247	-1.2698537
C	4.0636567	1.1724227	-0.5804564
Br	0.9456622	8.1694988	1.0778074
C	0.4505346	3.8249008	1.4885042
C	-0.6592248	2.8123055	1.2126152
C	0.0421147	5.1813023	1.8148844
C	1.6086617	3.2528676	2.3214677
C	2.8696580	3.0526371	1.4470453
O	3.8051657	4.1211396	1.5250709
H	3.4269938	2.1566122	1.7794405
H	1.8534494	3.9098406	3.1781808
H	1.2989420	2.2709818	2.7346305
H	0.4298502	5.6305106	2.7428872
H	-0.9780875	5.5078944	1.5500369
H	-1.1569939	2.5858423	2.1804241
H	-0.2514452	1.8695049	0.7983173
H	-1.4312899	3.1943898	0.5217889
H	3.3289182	4.9234004	1.1764542
H	0.8222130	1.3232123	-1.6850621
H	1.5621159	-0.7117558	-2.9080704
H	3.9166189	-1.5529527	-2.6599382
H	5.5102471	-0.3416338	-1.1422054
H	4.7725615	1.7036037	0.0716597
H	-1.1717275	4.8867052	-0.6299020
H	-2.2827518	5.4283290	-2.7651815
H	-1.1395238	4.9411071	-4.9544820
H	1.1481674	3.8896369	-4.9365703
H	2.2464483	3.3123122	-2.8010854
Pd	1.4313408	5.8347917	0.3938697
P	3.0936065	6.6202522	-1.0663273
C	2.4226704	7.9706966	-2.1080072
C	3.1175761	9.1700179	-2.3449684
H	4.0963206	9.3400787	-1.8731220
C	2.5511548	10.1526586	-3.1736533
H	3.0922890	11.0948397	-3.3493087
C	1.2983988	9.9379153	-3.7709829

H	0.8572577	10.7112118	-4.4182218
C	0.6034226	8.7392955	-3.5315263
H	-0.3834153	8.5683038	-3.9874796
C	1.1568129	7.7616530	-2.6943270
H	0.6028687	6.8344851	-2.4869489
C	4.5853641	7.3127876	-0.2406860
C	5.8128726	7.4057424	-0.9327373
H	5.8846243	7.0524466	-1.9720110
C	6.9425339	7.9389168	-0.2943656
H	7.8958249	8.0076100	-0.8402862
C	6.8577965	8.3783047	1.0378977
H	7.7467171	8.7909520	1.5391236
C	5.6384218	8.2863915	1.7283956
H	5.5658970	8.6284926	2.7717703
C	4.5036953	7.7560703	1.0952135
H	3.5398308	7.7028368	1.6245095
C	3.8456271	5.4824593	-2.2973072
C	3.6869330	5.6616890	-3.6859380
H	3.1248699	6.5265904	-4.0649888
C	4.2304598	4.7288237	-4.5829193
H	4.0973820	4.8735463	-5.6659518
C	4.9373446	3.6153530	-4.1005082
H	5.3575984	2.8796194	-4.8027386
C	5.1129474	3.4450796	-2.7162596
H	5.6680729	2.5761520	-2.3369437
C	4.5671768	4.3692546	-1.8138584
H	4.6893123	4.2295489	-0.7281674

S4

75

SCF Energy = -4548.281344605

C	1.4654681	3.9525342	-2.7314229
C	0.9351189	3.8759723	-1.4144440
C	-0.4299358	4.2379850	-1.2213582
C	-1.1989543	4.7247009	-2.2910453
C	-0.6417414	4.8379071	-3.5744261
C	0.6892301	4.4348600	-3.7883092
C	1.7376351	3.3076829	-0.2972830
C	2.2646704	2.0534984	-0.3258281
C	2.2920565	1.1591766	-1.5112863
C	1.1634608	0.9354448	-2.3321139
C	1.2497254	0.0837857	-3.4419299
C	2.4596398	-0.5608802	-3.7521900
C	3.5794487	-0.3674152	-2.9269026
C	3.4951110	0.4775819	-1.8103532
Br	0.4502482	7.7052456	0.9964287

C	1.9154921	3.7418562	1.6767719
C	3.2636277	4.3811703	2.0861355
C	0.7521570	4.5879785	1.9563500
C	1.8988699	2.2511885	2.0186011
C	2.7552466	1.4865145	0.9958348
O	4.1702098	1.5577049	1.1922095
H	2.5300636	0.4015161	1.0403423
H	2.2758312	2.1082324	3.0535667
H	0.8630874	1.8614506	1.9691006
H	-0.2436473	4.1184358	1.8750103
H	0.8300127	5.3343341	2.7637925
H	4.0549860	4.2603074	1.3198058
H	3.6358889	3.9155163	3.0235833
H	3.1719592	5.4734613	2.2437102
H	4.4337016	2.4828859	1.0312079
H	0.2116849	1.4292080	-2.0935816
H	0.3607357	-0.0800194	-4.0698082
H	2.5247265	-1.2234611	-4.6285617
H	4.5264395	-0.8825088	-3.1500977
H	4.3608720	0.6210371	-1.1470523
H	-0.8932103	4.1122504	-0.2345805
H	-2.2445789	5.0156983	-2.1115979
H	-1.2448070	5.2258656	-4.4088377
H	1.1320937	4.4943727	-4.7936214
H	2.4881613	3.6079425	-2.9150769
Pd	1.5017794	5.5969322	0.2762772
P	3.0718172	6.6787348	-1.1122655
C	4.4089060	7.4837138	-0.1323434
C	4.0599168	8.1593260	1.0575943
H	3.0020788	8.1975684	1.3672822
C	5.0533916	8.7822634	1.8272063
H	4.7715138	9.3080893	2.7521652
C	6.3993924	8.7331980	1.4249554
H	7.1768548	9.2178193	2.0351027
C	6.7496823	8.0633212	0.2413966
H	7.8013046	8.0235569	-0.0814403
C	5.7601007	7.4415019	-0.5373806
H	6.0394956	6.9177240	-1.4632305
C	4.0160996	5.5990098	-2.2600868
C	4.0174871	5.7927104	-3.6550037
H	3.5268790	6.6792162	-4.0818668
C	4.6107485	4.8382063	-4.4982109
H	4.5930963	4.9895182	-5.5882387
C	5.2117683	3.6898373	-3.9577142
H	5.6576523	2.9337900	-4.6208387
C	5.2386783	3.5054655	-2.5634217

H	5.7065775	2.6083919	-2.1337356
C	4.6418542	4.4526477	-1.7224445
H	4.6294242	4.2889899	-0.6353227
C	2.4111243	7.9970661	-2.1944126
C	3.1888326	9.0955404	-2.6100378
H	4.2214552	9.2060129	-2.2456203
C	2.6398887	10.0478787	-3.4830106
H	3.2455503	10.9090345	-3.8040572
C	1.3186924	9.9045103	-3.9416392
H	0.8901520	10.6545794	-4.6238687
C	0.5413497	8.8124724	-3.5197747
H	-0.4976102	8.7043138	-3.8656003
C	1.0807819	7.8632768	-2.6395695
H	0.4724814	7.0186929	-2.2847752

Optimized Geometries(BXnd/d')-exo

R1
75
SCF Energy = -4548.347409027

C	-0.3922850	3.3506488	-1.6713277
C	-0.2743158	1.9449217	-1.6431824
C	-1.3922264	1.1877227	-1.2150279
C	-2.5774336	1.8121701	-0.8044314
C	-2.6662871	3.2136709	-0.8076562
C	-1.5748010	3.9770782	-1.2497725
C	0.9826574	1.2456085	-2.0027587
C	1.1373363	0.2969677	-2.9757863
C	0.1436565	-0.1778475	-3.9567894
C	0.2637181	-1.4804512	-4.5034424
C	-0.6673922	-1.9583952	-5.4369997
C	-1.7367589	-1.1481950	-5.8524913
C	-1.8551931	0.1541540	-5.3355359
C	-0.9268130	0.6361651	-4.4040895
Br	0.4737417	3.4985057	1.9219334
C	2.2613475	1.4188479	-1.1533444
C	2.6849450	2.8771592	-0.9230570
C	2.1187242	0.6505278	0.1773677
C	3.3170405	0.6769913	-2.0354668
C	2.5330421	-0.3143521	-2.9135163
O	2.5219415	-1.6565821	-2.4067215
H	2.9861117	-0.4039382	-3.9234922
H	3.8169048	1.4286768	-2.6803099

H	4.1027901	0.1608409	-1.4493605
H	2.1460990	-0.4410564	-0.0000678
H	2.9089027	0.9257766	0.9068841
H	2.7797830	3.4145132	-1.8880942
H	3.6756143	2.8980020	-0.4240569
H	1.9747914	3.4209189	-0.2714455
H	1.8679341	-1.6896535	-1.6802899
H	1.0870270	-2.1211624	-4.1577408
H	-0.5551346	-2.9754092	-5.8443128
H	-2.4679576	-1.5234765	-6.5846509
H	-2.6764244	0.8070112	-5.6688954
H	-1.0206666	1.6628330	-4.0262176
H	-1.3185746	0.0945534	-1.2428703
H	-3.4256297	1.1992834	-0.4657708
H	-3.5865667	3.7110733	-0.4665601
H	-1.6379924	5.0751645	-1.2582654
H	0.4518632	3.9606041	-2.0170917
Pd	0.4047070	1.1773659	1.1646730
P	-0.1852227	-0.9681160	1.4024347
C	-1.9966907	-0.9922250	1.7224764
C	-2.5790639	0.1968832	2.2120905
H	-1.9582594	1.0980006	2.3583250
C	-3.9501961	0.2434300	2.5030425
H	-4.3937667	1.1770384	2.8796447
C	-4.7502093	-0.8944563	2.3057932
H	-5.8271686	-0.8565617	2.5289405
C	-4.1743055	-2.0816801	1.8221256
H	-4.7980723	-2.9750748	1.6676178
C	-2.8019025	-2.1342457	1.5327759
H	-2.3602988	-3.0649370	1.1474408
C	0.0950705	-2.2848134	0.1527784
C	1.2326855	-3.1186757	0.2508661
H	1.9206922	-3.0083930	1.1016974
C	1.4805683	-4.0961167	-0.7262390
H	2.3740353	-4.7318920	-0.6430260
C	0.6039394	-4.2485588	-1.8117595
H	0.8065438	-5.0082105	-2.5808684
C	-0.5209403	-3.4150294	-1.9244239
H	-1.2025083	-3.5124776	-2.7810366
C	-0.7723031	-2.4358525	-0.9530777
H	-1.6640331	-1.8011552	-1.0497183
C	0.5530981	-1.6796894	2.9318674
C	1.4632256	-0.9019889	3.6735473
H	1.7135385	0.1102453	3.3138627
C	2.0207987	-1.4123074	4.8577138
H	2.7308784	-0.7998818	5.4333373

C	1.6685949	-2.6954733	5.3046191
H	2.1043966	-3.0946145	6.2330899
C	0.7543508	-3.4716519	4.5686565
H	0.4736073	-4.4758271	4.9207514
C	0.1957247	-2.9670216	3.3864150
H	-0.5186069	-3.5772559	2.8136816

R2(d')

75

SCF Energy = -4548.350329009

C	1.3167660	-0.8129386	-1.5888877
C	1.6039153	-1.8354948	-0.6506412
C	1.3451066	-3.1732670	-1.0226760
C	0.8102155	-3.4776393	-2.2863246
C	0.5144685	-2.4509768	-3.1974204
C	0.7732243	-1.1145454	-2.8426183
C	2.1136243	-1.4577183	0.6922732
C	3.1422914	-0.5841548	0.9306617
C	4.0398467	0.0316191	-0.0626441
C	4.5687648	-0.7217142	-1.1382889
C	5.4171494	-0.1243222	-2.0789793
C	5.7517770	1.2368529	-1.9646456
C	5.2368815	1.9932011	-0.8987304
C	4.3941277	1.3967488	0.0504026
Br	1.0859947	2.6529975	1.1804330
C	1.4431670	-1.9258302	2.0144144
C	1.7410863	-3.3945023	2.3775252
C	-0.0475274	-1.6319519	1.8573745
C	2.0950920	-0.9546584	3.0560489
C	3.3764207	-0.4041356	2.4235127
O	4.4910457	-1.1981470	2.8527221
H	3.5344660	0.6674054	2.6881618
H	1.4048995	-0.1017249	3.2677141
H	2.3056251	-1.4411684	4.0282043
H	-0.6185902	-1.6387956	2.8096405
H	-0.5339079	-2.2859647	1.1125458
H	1.3146873	-3.6289554	3.3741917
H	2.8376449	-3.5538579	2.4193368
H	1.2947035	-4.1023882	1.6529493
H	5.2365927	-0.9724011	2.2633923
H	4.3074023	-1.7863092	-1.2251933
H	5.8229616	-0.7249365	-2.9073543
H	6.4160486	1.7064223	-2.7062097
H	5.4866383	3.0612590	-0.8079212
H	3.9545976	2.0010336	0.8573448
H	1.5752027	-3.9875592	-0.3231075

H	0.6201136	-4.5277942	-2.5561531
H	0.0793732	-2.6885555	-4.1798391
H	0.5294915	-0.2970091	-3.5368104
H	1.5011229	0.2330920	-1.3039186
Pd	0.1693463	0.3256208	1.2567600
P	-1.7949934	0.3592082	0.2520227
C	-2.9618162	1.5504483	1.0156122
C	-1.6817780	0.9060975	-1.5045420
C	-2.7112890	-1.2230828	0.1657518
C	-4.1937982	1.8391934	0.3909208
C	-5.0799766	2.7486660	0.9847656
C	-4.7378135	3.3776356	2.1957184
C	-3.5069503	3.0989583	2.8107121
C	-2.6158071	2.1872141	2.2220307
H	-4.4557347	1.3566726	-0.5630547
H	-6.0402134	2.9742850	0.4966598
H	-5.4332626	4.0957978	2.6561922
H	-3.2308354	3.6001675	3.7504200
H	-1.6336610	1.9776024	2.6745389
C	-2.5037599	0.3483639	-2.5061153
C	-2.3970671	0.7962448	-3.8324124
C	-1.4778016	1.8039684	-4.1663751
C	-0.6701741	2.3709142	-3.1650479
C	-0.7678652	1.9268849	-1.8385895
H	-3.2212327	-0.4459987	-2.2568931
H	-3.0364428	0.3499316	-4.6091224
H	-1.3904898	2.1476839	-5.2083489
H	0.0521472	3.1619845	-3.4166869
H	-0.1203377	2.3594964	-1.0566342
C	-3.8198017	-1.4862758	0.9928735
C	-4.4217353	-2.7559807	0.9752685
C	-3.9198951	-3.7659165	0.1387748
C	-2.8053475	-3.5076296	-0.6794676
C	-2.1966829	-2.2463010	-0.6625502
H	-4.2138266	-0.6974896	1.6504902
H	-5.2901022	-2.9548100	1.6214364
H	-4.3942834	-4.7588726	0.1280219
H	-2.3965693	-4.2946441	-1.3308558
H	-1.3152487	-2.0562638	-1.2923903

R3(d')

75

SCF Energy = -4548.348159889

C	-1.0172138	2.3499909	-1.1522557
C	-1.3207521	1.5002420	-2.2374903
C	-1.4870476	2.0699671	-3.5185992

C	-1.3495124	3.4527056	-3.7077050
C	-1.0410935	4.2888012	-2.6214059
C	-0.8747803	3.7321208	-1.3425574
C	-1.4874037	0.0293263	-2.0857386
C	-0.7196616	-0.9473302	-2.7212104
C	0.4110163	-0.6460278	-3.6269442
C	0.5181851	-1.2847687	-4.8857337
C	1.5452335	-0.9428249	-5.7801331
C	2.4795991	0.0474347	-5.4425340
C	2.3739782	0.7014550	-4.2027296
C	1.3570673	0.3588366	-3.3064975
Br	2.1473735	-1.4504168	-0.6690144
C	-2.7556538	-0.5823580	-1.4257344
C	-4.0333877	0.2267913	-1.6570925
C	-2.3041499	-0.6206214	0.0291572
C	-2.8023064	-1.9873795	-2.0737006
C	-1.3773320	-2.3389371	-2.5307072
O	-1.4546449	-3.1666476	-3.6879296
H	-0.8134607	-2.8864777	-1.7370061
H	-3.2419905	-2.7522940	-1.4037563
H	-3.4171908	-1.9474816	-2.9969957
H	-2.5993180	-1.5192298	0.6092187
H	-2.5791258	0.2942654	0.5833115
H	-4.2462928	0.3386601	-2.7405764
H	-3.9462898	1.2415616	-1.2204359
H	-4.8987116	-0.2799098	-1.1823001
H	-0.5836425	-3.5935518	-3.7909025
H	-0.2447226	-2.0168527	-5.1779118
H	1.6035240	-1.4491859	-6.7559039
H	3.2851788	0.3137354	-6.1437604
H	3.1007146	1.4790575	-3.9234325
H	1.2952631	0.8605764	-2.3339038
H	-1.7097462	1.4122909	-4.3716947
H	-1.4753616	3.8793251	-4.7144313
H	-0.9229901	5.3723824	-2.7737697
H	-0.6167982	4.3730297	-0.4859027
H	-0.8485420	1.9047492	-0.1614235
Pd	-0.2621466	-0.7566016	-0.2813745
P	0.1863576	-0.3917055	1.8990865
C	1.0804496	1.2011668	2.1152390
C	1.8895460	1.6840227	1.0652077
H	1.9974462	1.0815484	0.1495897
C	2.5674103	2.9040717	1.2072001
H	3.1925140	3.2738969	0.3807198
C	2.4484344	3.6481468	2.3926226
H	2.9777915	4.6073468	2.4986003

C	1.6522465	3.1652158	3.4449979
H	1.5587005	3.7412808	4.3781077
C	0.9682605	1.9473037	3.3095486
H	0.3342056	1.5826161	4.1308273
C	1.1779488	-1.6796382	2.7455221
C	1.0770122	-3.0098390	2.2919356
H	0.4814847	-3.2286150	1.3929571
C	1.7581797	-4.0327158	2.9674965
H	1.6803489	-5.0697153	2.6081275
C	2.5561285	-3.7293145	4.0837602
H	3.1007631	-4.5310799	4.6051745
C	2.6698672	-2.4008060	4.5262864
H	3.3044534	-2.1588902	5.3922430
C	1.9796117	-1.3748850	3.8618832
H	2.0768554	-0.3344498	4.2050843
C	-1.2780388	-0.2088448	2.9948236
C	-1.6998720	-1.2693418	3.8210841
H	-1.0963159	-2.1867690	3.8838072
C	-2.8816863	-1.1536094	4.5712269
H	-3.1985684	-1.9862698	5.2172774
C	-3.6511370	0.0186848	4.5040566
H	-4.5749180	0.1083356	5.0952284
C	-3.2369521	1.0786774	3.6787640
H	-3.8351163	2.0005029	3.6198868
C	-2.0620220	0.9645713	2.9228307
H	-1.7427594	1.7993558	2.2803259

R4

75

SCF Energy = -4548.344829393

C	-0.2109747	-6.3224073	1.4091955
C	-0.3187460	-5.2067480	0.5404480
C	-0.1659142	-5.4328635	-0.8512050
C	0.1135179	-6.7123074	-1.3472096
C	0.2423835	-7.8032532	-0.4701905
C	0.0732312	-7.6008845	0.9091229
C	-0.5881962	-3.8673349	1.0912181
Pd	0.1226289	0.2873189	-0.6674065
P	-0.4511429	2.4299228	-0.4718091
C	-0.3034584	-2.6499088	0.5457595
Br	2.2243808	0.9754939	-1.9079701
C	0.3749353	-2.3613369	-0.7410968
C	1.7517216	-2.6539891	-0.9239812
C	2.3471919	-2.5142321	-2.1795671
C	1.5875452	-2.0879511	-3.2869392
C	0.2323056	-1.7840802	-3.1308441

C	-0.3798421	-1.8979822	-1.8625349
C	-1.2257270	-3.6741538	2.4728805
O	-2.2673081	-4.5858151	2.7923783
C	-1.6637939	-2.1918079	2.4501426
C	-0.6857825	-1.4929471	1.4684716
C	-1.3110871	-0.3292858	0.6925174
C	0.5803893	-1.0044217	2.2194257
H	-0.4593581	-3.8425885	3.2640539
H	-1.6912004	-1.7240148	3.4538389
H	-2.6918221	-2.1559071	2.0299908
H	-2.2267979	-0.6390135	0.1434191
H	-1.5916890	0.4818989	1.3908132
H	0.3301619	-0.1357127	2.8624925
H	1.3653748	-0.6802927	1.5037684
H	1.0085797	-1.8038877	2.8572786
H	-2.8511799	-4.6320449	2.0106340
H	-0.2807302	-4.5983850	-1.5551067
H	0.2270568	-6.8594028	-2.4321750
H	0.4625535	-8.8079638	-0.8618915
H	0.1585171	-8.4491187	1.6055761
H	-0.3696076	-6.1848149	2.4868260
H	-1.4681179	-1.7776314	-1.7669369
H	-0.3657041	-1.4460145	-3.9896260
H	2.0668486	-1.9765527	-4.2700058
H	3.4176376	-2.7335917	-2.3025615
H	2.3345833	-3.0090446	-0.0622168
C	-0.9668642	3.2097919	-2.0573367
C	0.8872292	3.4768070	0.2160235
C	-1.8830187	2.8015794	0.6214937
C	-1.7261034	3.4453530	1.8635779
C	-2.8394146	3.6427719	2.6986969
C	-4.1105668	3.2024785	2.2990756
C	-4.2697510	2.5572421	1.0589845
C	-3.1622437	2.3512465	0.2269574
H	-0.7318731	3.7952579	2.1771927
H	-2.7091245	4.1486482	3.6673441
H	-4.9805857	3.3592681	2.9543823
H	-5.2638687	2.2073583	0.7420749
H	-3.2837607	1.8357297	-0.7382659
C	-1.8390656	4.3218356	-2.0478818
C	-2.2074250	4.9368686	-3.2541390
C	-1.7150998	4.4457784	-4.4750294
C	-0.8504244	3.3390173	-4.4853708
C	-0.4747679	2.7189626	-3.2836639
H	-2.2369093	4.7036764	-1.0963519
H	-2.8857328	5.8034510	-3.2382069

H	-2.0088152	4.9269805	-5.4204420
H	-0.4603609	2.9509009	-5.4384516
H	0.2232727	1.8665388	-3.2799240
C	1.7669133	2.8976686	1.1524326
C	2.7615092	3.6797712	1.7555980
C	2.8938788	5.0367004	1.4134670
C	2.0269215	5.6102894	0.4689057
C	1.0207470	4.8347672	-0.1289857
H	1.6745801	1.8262578	1.3854048
H	3.4487010	3.2225735	2.4831994
H	3.6836872	5.6468913	1.8773324
H	2.1369931	6.6688951	0.1889290
H	0.3489450	5.2837593	-0.8750482

S1

75

SCF Energy = -4548.346217859

C	-0.4947448	1.8316805	-2.7552077
C	-0.6085071	0.4667821	-2.3861290
C	-1.8562902	0.0001873	-1.8687824
C	-2.9565841	0.8813107	-1.7704782
C	-2.8196631	2.2209952	-2.1438835
C	-1.5851323	2.6956313	-2.6289300
C	0.4917308	-0.4938613	-2.6450838
C	0.9004176	-0.9855404	-3.8508618
C	0.3579241	-0.7035827	-5.1927474
C	-0.9899523	-0.3158740	-5.3966976
C	-1.4779741	-0.0674585	-6.6861284
C	-0.6366119	-0.1994946	-7.8042930
C	0.6996174	-0.5904395	-7.6188876
C	1.1921753	-0.8425895	-6.3306861
Br	-1.2269402	2.6729231	0.8720285
C	1.3305104	-1.0135787	-1.4770794
C	2.3281672	0.0832684	-1.0217207
C	0.4443823	-1.4197759	-0.2925979
C	2.0743937	-2.2094015	-2.1363905
C	2.1135953	-1.8932470	-3.6498309
O	3.3319263	-1.2709341	-4.0901376
H	2.0407946	-2.8179012	-4.2597715
H	3.0912530	-2.3775127	-1.7305870
H	1.4841014	-3.1350591	-1.9760431
H	-0.2954582	-2.2002974	-0.5722865
H	1.0711425	-1.8218001	0.5263527
H	1.8019258	1.0241754	-0.7540952
H	3.0655966	0.3140144	-1.8168723
H	2.8870713	-0.2594310	-0.1269516

H	3.2788465	-0.3336366	-3.8210129
H	-1.6693091	-0.2275560	-4.5387703
H	-2.5302702	0.2270841	-6.8191367
H	-1.0230154	-0.0021456	-8.8158174
H	1.3685643	-0.6978999	-8.4866155
H	2.2449870	-1.1234639	-6.1822014
H	-1.9993053	-1.0753941	-1.6947097
H	-3.9166379	0.5037483	-1.3894845
H	-3.6705241	2.9100205	-2.0441100
H	-1.4769407	3.7540733	-2.9065541
H	0.4636391	2.1930358	-3.1546063
Pd	-0.5461478	0.3060846	0.2795508
P	-0.5385946	-0.2712593	2.4287729
C	-2.2230491	-0.3679496	3.1651207
C	-3.2629897	0.4384127	2.6590510
H	-3.0538729	1.1227982	1.8208897
C	-4.5369753	0.3840674	3.2450445
H	-5.3427621	1.0182546	2.8454485
C	-4.7845718	-0.4704010	4.3320207
H	-5.7865665	-0.5120930	4.7857692
C	-3.7499824	-1.2747952	4.8384148
H	-3.9363971	-1.9465854	5.6900494
C	-2.4730284	-1.2280109	4.2583082
H	-1.6703755	-1.8678509	4.6530300
C	0.1606811	-1.9232003	2.8311799
C	1.3861104	-2.0684645	3.5088124
H	1.9218782	-1.1778708	3.8682005
C	1.9206544	-3.3499165	3.7275394
H	2.8780728	-3.4558661	4.2597509
C	1.2365764	-4.4885363	3.2746013
H	1.6568994	-5.4906189	3.4481174
C	0.0128999	-4.3459159	2.5950800
H	-0.5258274	-5.2353842	2.2349831
C	-0.5198093	-3.0708313	2.3677341
H	-1.4714287	-2.9574945	1.8257397
C	0.4272211	0.8687223	3.4904240
C	1.5329749	1.5325615	2.9230600
H	1.7388328	1.4107763	1.8490933
C	2.3387601	2.3574168	3.7204057
H	3.1987820	2.8773842	3.2725664
C	2.0336877	2.5366432	5.0806190
H	2.6589033	3.1947843	5.7029153
C	0.9224028	1.8867743	5.6430045
H	0.6737748	2.0359237	6.7046508
C	0.1190482	1.0502178	4.8520608
H	-0.7556173	0.5491213	5.2919495

S2(d')

75

SCF Energy = -4548.360809179

C	-2.5213938	-1.1567697	-1.0791237
C	-1.6883068	-1.6875477	-2.0867518
C	-2.2865737	-2.2523133	-3.2347883
C	-3.6822110	-2.2777596	-3.3719105
C	-4.5027479	-1.7424303	-2.3643865
C	-3.9171499	-1.1814304	-1.2175636
C	-0.2046471	-1.7163658	-1.9790614
C	0.7239974	-0.9442681	-2.6900140
C	0.4545440	0.1700120	-3.6197037
C	-0.8021333	0.8214481	-3.6832553
C	-1.0226500	1.8723390	-4.5787767
C	0.0059777	2.3132598	-5.4293921
C	1.2642588	1.6970927	-5.3611384
C	1.4862915	0.6420453	-4.4655340
Br	1.2488056	2.0705987	-1.0356225
C	0.4945347	-2.8928155	-1.2331117
C	-0.2369376	-4.2334353	-1.3173586
C	0.5110437	-2.2920859	0.1665255
C	1.8892881	-2.9223911	-1.9081165
C	2.1273133	-1.5474310	-2.5652151
O	3.0224979	-0.7408468	-1.7930589
H	2.5620333	-1.6886776	-3.5824969
H	2.7036133	-3.1644877	-1.1980793
H	1.8855894	-3.7022434	-2.6968107
H	1.4293524	-2.4676104	0.7622353
H	-0.3920522	-2.5386373	0.7531574
H	0.3266983	-5.0082404	-0.7579826
H	-0.3404314	-4.5728297	-2.3691864
H	-1.2527908	-4.1640923	-0.8800701
H	2.6789463	0.1874115	-1.7797775
H	-1.6072896	0.5196288	-3.0036675
H	-2.0073120	2.3633756	-4.6031729
H	-0.1688326	3.1447061	-6.1288940
H	2.0870161	2.0452848	-6.0037079
H	2.4872836	0.1924994	-4.4104960
H	-1.6434963	-2.6568514	-4.0306516
H	-4.1325239	-2.7142192	-4.2763881
H	-5.5973757	-1.7573860	-2.4770905
H	-4.5476042	-0.7467762	-0.4271186
H	-2.0486215	-0.6892854	-0.2025897
Pd	0.5584114	-0.2934775	-0.3608854
P	0.2237131	0.3704092	1.7732967

C	-1.2887908	1.3951308	1.9656345
C	-1.8022822	2.0891712	0.8501460
H	-1.2746858	2.0267530	-0.1146101
C	-2.9635797	2.8656540	0.9834916
H	-3.3577347	3.4029922	0.1079161
C	-3.6178438	2.9565764	2.2230629
H	-4.5301399	3.5642926	2.3228904
C	-3.1078087	2.2677269	3.3368728
H	-3.6172831	2.3346725	4.3101636
C	-1.9492150	1.4863957	3.2111923
H	-1.5650951	0.9324762	4.0806153
C	-0.0334396	-0.9772810	2.9947410
C	0.9996255	-1.3889688	3.8590902
H	1.9530353	-0.8405474	3.8716537
C	0.8107822	-2.4919875	4.7085554
H	1.6222946	-2.8025161	5.3839555
C	-0.4061974	-3.1914367	4.7010385
H	-0.5523084	-4.0535668	5.3691100
C	-1.4384319	-2.7877068	3.8356504
H	-2.3942179	-3.3330324	3.8223080
C	-1.2524591	-1.6916764	2.9822304
H	-2.0629585	-1.3812116	2.3047838
C	1.6296198	1.3162904	2.4675292
C	2.9180949	1.0289297	1.9718644
H	3.0324494	0.3145893	1.1414951
C	4.0357878	1.6763342	2.5178803
H	5.0393697	1.4528729	2.1262906
C	3.8698708	2.6232079	3.5430770
H	4.7466721	3.1405503	3.9613748
C	2.5840361	2.9210259	4.0248839
H	2.4514517	3.6723827	4.8180430
C	1.4622366	2.2668131	3.4918468
H	0.4554795	2.5076608	3.8636728

S3(d')

75

SCF Energy = -4548.360809395

C	-2.5180354	-1.1636736	-1.0771955
C	-1.6844830	-1.6915355	-2.0859785
C	-2.2822909	-2.2569373	-3.2339424
C	-3.6779739	-2.2858173	-3.3698907
C	-4.4989948	-1.7533357	-2.3612504
C	-3.9138411	-1.1917616	-1.2144843
C	-0.2006685	-1.7166124	-1.9795663
C	0.7252424	-0.9423101	-2.6914721
C	0.4520427	0.1711733	-3.6209927

C	-0.8060332	0.8201285	-3.6824553
C	-1.0302725	1.8702329	-4.5779726
C	-0.0040621	2.3128667	-5.4306191
C	1.2555644	1.6992282	-5.3644328
C	1.4813114	0.6449374	-4.4688535
Br	1.2415285	2.0744621	-1.0370428
C	0.5021469	-2.8909168	-1.2336740
C	-0.2256385	-4.2335901	-1.3176144
C	0.5177781	-2.2904457	0.1661080
C	1.8966745	-2.9166378	-1.9093689
C	2.1303920	-1.5411513	-2.5668576
O	3.0230874	-0.7316469	-1.7948140
H	2.5655571	-1.6812770	-3.5840953
H	2.7120608	-3.1562705	-1.1997207
H	1.8947808	-3.6965901	-2.6979702
H	1.4366255	-2.4643358	0.7614674
H	-0.3845318	-2.5393053	0.7530103
H	-0.3283102	-4.5735028	-2.3693611
H	-1.2416194	-4.1669895	-0.8801978
H	0.3402005	-5.0067087	-0.7581216
H	2.6771728	0.1957447	-1.7824673
H	-1.6092954	0.5169878	-3.0012114
H	-2.0159306	2.3593488	-4.6007034
H	-0.1817628	3.1437266	-6.1300905
H	2.0764531	2.0488239	-6.0086229
H	2.4832578	0.1973083	-4.4156371
H	-1.6388726	-2.6592468	-4.0306598
H	-4.1279441	-2.7227335	-4.2743203
H	-5.5936804	-1.7709754	-2.4730018
H	-4.5447446	-0.7593657	-0.4231585
H	-2.0456209	-0.6957239	-0.2007077
Pd	0.5598918	-0.2916501	-0.3608513
P	0.2264154	0.3706514	1.7736099
C	-1.2883687	1.3913796	1.9689010
C	-1.8061494	2.0836021	0.8542708
H	-1.2805310	2.0221226	-0.1116155
C	-2.9691395	2.8571601	0.9898747
H	-3.3666590	3.3930701	0.1149447
C	-3.6208625	2.9469392	2.2308639
H	-4.5344839	3.5523649	2.3324715
C	-3.1065959	2.2598537	3.3438181
H	-3.6140441	2.3259422	4.3182255
C	-1.9462795	1.4814516	3.2158808
H	-1.5588474	0.9288460	4.0846703
C	1.6311680	1.3197040	2.4659918
C	2.9193012	1.0370995	1.9667069

H	3.0337509	0.3244333	1.1349130
C	4.0363418	1.6870430	2.5110578
H	5.0396371	1.4672901	2.1166441
C	3.8700499	2.6316929	3.5382326
H	4.7462834	3.1510386	3.9552391
C	2.5844970	2.9247430	4.0237142
H	2.4515562	3.6743696	4.8184493
C	1.4634071	2.2679809	3.4923295
H	0.4568485	2.5051825	3.8670127
C	-0.0251554	-0.9784163	2.9946677
C	1.0115372	-1.3897229	3.8548588
H	1.9641553	-0.8398569	3.8648860
C	0.8273182	-2.4941602	4.7034735
H	1.6416168	-2.8043377	5.3756764
C	-0.3886211	-3.1954573	4.6992206
H	-0.5311029	-4.0587138	5.3666225
C	-1.4244415	-2.7921443	3.8379427
H	-2.3794019	-3.3389700	3.8270944
C	-1.2430976	-1.6946715	2.9853701
H	-2.0563213	-1.3846446	2.3110020

S4

75

SCF Energy = -4548.346204019

C	-0.1069724	2.7009164	-1.9112145
C	0.4617814	2.3805340	-0.6518258
C	1.8036324	1.8904010	-0.6124170
C	2.5499910	1.7718942	-1.8063367
C	1.9680713	2.0977145	-3.0343783
C	0.6365352	2.5550096	-3.0846864
C	-0.2596743	2.6665910	0.6123094
C	-0.5024795	3.8863219	1.1745692
C	-0.1116245	5.2214559	0.6857275
C	-0.8713153	6.3573050	1.0638832
C	-0.5166791	7.6396202	0.6217542
C	0.6058264	7.8213351	-0.2026337
C	1.3741229	6.7055516	-0.5773549
C	1.0225435	5.4218932	-0.1401988
Br	0.4165496	-0.9509506	-2.8409649
C	-0.8540833	1.5122117	1.4190225
C	-2.1537604	1.0131360	0.7357296
C	0.1384302	0.3486306	1.5389563
C	-1.1654876	2.2078329	2.7742900
C	-1.3370881	3.7087066	2.4427770
O	-2.7017009	4.1177509	2.2524825
H	-0.9699166	4.3518141	3.2697705

H	-2.0589459	1.8009537	3.2872298
H	-0.2955007	2.0850626	3.4518857
H	1.0927164	0.6616348	2.0152141
H	-0.3021682	-0.4571313	2.1559612
H	-2.9419165	1.7928643	0.7479443
H	-2.5458200	0.1231190	1.2690850
H	-1.9693078	0.7230300	-0.3204326
H	-2.9614297	3.8148952	1.3610656
H	-1.7648913	6.2107014	1.6878011
H	-1.1262252	8.5055669	0.9227290
H	0.8841412	8.8283126	-0.5490127
H	2.2628307	6.8361355	-1.2136679
H	1.6482797	4.5665766	-0.4270478
H	2.2999385	1.7549650	0.3586677
H	3.5883225	1.4126538	-1.7592022
H	2.5432250	1.9819131	-3.9640772
H	0.1770863	2.7952245	-4.0543899
H	-1.1384152	3.0797914	-1.9441212
Pd	0.5115764	-0.2783489	-0.3991631
P	0.6404155	-2.4201742	0.1965129
C	-0.6552541	-3.4669375	-0.5691352
C	-1.9092371	-2.8831793	-0.8384078
H	-2.0515370	-1.8077160	-0.6550543
C	-2.9489715	-3.6663013	-1.3586750
H	-3.9251918	-3.2054213	-1.5712740
C	-2.7360810	-5.0290641	-1.6291540
H	-3.5486810	-5.6402434	-2.0503527
C	-1.4816327	-5.6076768	-1.3750669
H	-1.3080000	-6.6711699	-1.5986778
C	-0.4404241	-4.8309749	-0.8423374
H	0.5436634	-5.2839772	-0.6528807
C	0.4753512	-2.7867431	1.9909398
C	-0.6642622	-3.4220500	2.5196223
H	-1.4600789	-3.7691850	1.8447784
C	-0.7816816	-3.6143670	3.9070588
H	-1.6745948	-4.1135027	4.3129009
C	0.2347556	-3.1773246	4.7704101
H	0.1406412	-3.3301581	5.8561073
C	1.3737752	-2.5402987	4.2447518
H	2.1722028	-2.1927656	4.9176425
C	1.4916232	-2.3392338	2.8638078
H	2.3768494	-1.8297282	2.4526684
C	2.2544219	-3.2038037	-0.2139224
C	2.7203083	-4.3051045	0.5392178
H	2.1365948	-4.6766189	1.3940925
C	3.9346366	-4.9230494	0.2037357

H	4.2899022	-5.7810995	0.7944096
C	4.6931930	-4.4461821	-0.8784042
H	5.6475448	-4.9297949	-1.1371569
C	4.2315821	-3.3506626	-1.6263075
H	4.8204191	-2.9739089	-2.4763059
C	3.0175804	-2.7272872	-1.2991862
H	2.6360199	-1.8827924	-1.8955857

Optimized Geometries(MXnd)-exo

R3
75
SCF Energy = -4548.350665449

C	2.8075176	2.0689683	-0.1974133
C	1.8210211	1.6517857	-1.1168033
C	0.8152004	2.5849947	-1.4753772
C	0.8037283	3.8799724	-0.9454049
C	1.8050011	4.2826815	-0.0463753
C	2.8013351	3.3694795	0.3268120
C	1.8259323	0.3080160	-1.7452211
C	2.0961792	-0.9775268	-1.2058948
C	2.5265539	-1.4505501	0.1366792
C	3.7635723	-1.0838540	0.7074794
C	4.1942807	-1.6562282	1.9152912
C	3.4004097	-2.6152428	2.5656882
C	2.1905076	-3.0272076	1.9797592
C	1.7736770	-2.4647772	0.7669841
Br	-2.4384395	-1.2387751	-1.8364115
C	1.6741458	0.1138047	-3.3093155
C	2.0168341	1.3231682	-4.1756034
C	0.2237643	-0.3687544	-3.3968782
C	2.6155300	-1.0752254	-3.5571012
C	2.4326555	-1.9956294	-2.3444295
O	3.5488613	-2.8150970	-2.0606247
H	1.5926588	-2.7064442	-2.4825985
H	2.4231347	-1.5771370	-4.5265562
H	3.6698107	-0.7167811	-3.5549385
H	0.0553809	-1.3193270	-3.9355053
H	-0.5082322	0.3976417	-3.7146858
H	1.9810707	1.0377661	-5.2466667
H	3.0358776	1.7004393	-3.9491611
H	1.3092594	2.1605709	-4.0277667
H	4.3029034	-2.2280946	-1.8565748

H	4.4063348	-0.3535027	0.1951514
H	5.1563569	-1.3472490	2.3512282
H	3.7296441	-3.0501077	3.5212270
H	1.5586621	-3.7825697	2.4698938
H	0.8382722	-2.7990542	0.2981639
H	0.0207311	2.2743895	-2.1687840
H	0.0033932	4.5778563	-1.2338426
H	1.7995001	5.3001318	0.3720301
H	3.5810390	3.6645898	1.0437857
H	3.5945484	1.3719565	0.1068498
Pd	-0.1099843	-0.5792549	-1.3606024
P	-0.6868387	-0.1123689	0.9801855
C	-2.2803814	0.8144454	1.0020434
C	-2.5391486	1.7377326	-0.0311251
H	-1.8233766	1.8364600	-0.8589239
C	-3.7066209	2.5134461	-0.0105781
H	-3.9001441	3.2296790	-0.8233268
C	-4.6355395	2.3593179	1.0324696
H	-5.5586542	2.9586606	1.0422946
C	-4.3881751	1.4305964	2.0563463
H	-5.1167203	1.2992348	2.8708895
C	-3.2126946	0.6625936	2.0453429
H	-3.0234021	-0.0638530	2.8490581
C	-1.0235678	-1.5476415	2.0857342
C	-1.5461820	-2.7142551	1.4864413
H	-1.7620544	-2.7151291	0.4050894
C	-1.7916260	-3.8553345	2.2637292
H	-2.1955954	-4.7607787	1.7860414
C	-1.5198907	-3.8446741	3.6433511
H	-1.7052156	-4.7441166	4.2501688
C	-1.0177969	-2.6795310	4.2455986
H	-0.8132521	-2.6601503	5.3270183
C	-0.7738173	-1.5326328	3.4725705
H	-0.3779406	-0.6255561	3.9507003
C	0.3713105	0.9970775	2.0120579
C	0.0407315	2.3562474	2.1910073
H	-0.8634974	2.7686375	1.7234704
C	0.8569453	3.1873529	2.9732608
H	0.5819118	4.2448157	3.1037357
C	2.0133517	2.6790167	3.5842572
H	2.6480170	3.3334999	4.2009856
C	2.3521183	1.3279596	3.4037595
H	3.2537628	0.9093442	3.8760917
C	1.5401659	0.4938593	2.6238433
H	1.8026197	-0.5640406	2.5190166

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R4
75
SCF Energy = -4548.334216959
C      0.3647759   -2.2475880   -0.9838870
C     -0.4108382   -1.9754068    0.1847310
C     -1.7116136   -1.3818699    0.0162889
C     -2.2063326   -1.1331562   -1.2977976
C     -1.4431511   -1.4590643   -2.4146386
C     -0.1519489   -2.0177930   -2.2542560
C     -0.0201503   -2.5359085    1.5009041
C      0.2023245   -3.8387606    1.8353639
C      0.0679316   -5.0393644    0.9950690
C     -0.8515408   -5.0954856   -0.0823892
C     -0.9530614   -6.2399474   -0.8830675
C     -0.1466932   -7.3618556   -0.6232199
C      0.7507609   -7.3316448    0.4569526
C      0.8523902   -6.1887353    1.2624617
Br    -0.7639529    2.5913906    1.8750611
C      0.2498230   -1.5850835    2.6629798
C      1.6860485   -1.0126701    2.5282403
C     -0.7681884   -0.4459569    2.6518031
C      0.1728189   -2.5538055    3.8740321
C      0.6262763   -3.9224128    3.3088021
O      0.1292900   -5.0484730    4.0129763
H      1.7340497   -4.0220233    3.3764003
H      0.7637692   -2.2199008    4.7492350
H     -0.8860625   -2.6589336    4.1947336
H     -1.8132541   -0.7978721    2.7694585
H     -0.5585844    0.3266037    3.4141855
H      2.4506182   -1.8126254    2.5957228
H      1.8779267   -0.2686609    3.3276591
H      1.8168465   -0.4970868    1.5533996
H     -0.8274059   -5.1025529    3.8227596
H     -1.5066818   -4.2365302   -0.2821604
H     -1.6752776   -6.2590895   -1.7135185
H     -0.2280774   -8.2612979   -1.2522389
H      1.3756583   -8.2102140    0.6790385
H      1.5412741   -6.1852178    2.1178809
H     -2.4303033   -1.4051750    0.8459807
H     -3.2255634   -0.7355359   -1.4141442
H     -1.8391919   -1.2897027   -3.4255628
H      0.4427789   -2.2677957   -3.1429473
H      1.3558244   -2.7061128   -0.8555068
Pd    -0.5149897    0.4046237    0.7601701
P      0.2628729    1.6773306   -1.1456197
C     -0.9240470    3.0232704   -1.5482962

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C	-0.5465924	4.3628974	-1.7534499
H	0.5072555	4.6592162	-1.6561505
C	-1.5202450	5.3282158	-2.0561552
H	-1.2185771	6.3763261	-2.2040195
C	-2.8723399	4.9637859	-2.1606085
H	-3.6324406	5.7242966	-2.3953305
C	-3.2543723	3.6285854	-1.9457096
H	-4.3146662	3.3398165	-2.0054717
C	-2.2863492	2.6651923	-1.6289916
H	-2.5821856	1.6266469	-1.4179250
C	1.8730591	2.5090604	-0.7861317
C	2.4310776	2.4540815	0.5062149
H	1.8770406	1.9550305	1.3134113
C	3.6720028	3.0572010	0.7676933
H	4.0968430	3.0045177	1.7814202
C	4.3632378	3.7261931	-0.2543340
H	5.3344486	4.2007152	-0.0465710
C	3.8135882	3.7843262	-1.5469280
H	4.3518536	4.3034678	-2.3545466
C	2.5798775	3.1735288	-1.8144317
H	2.1682545	3.1996497	-2.8343296
C	0.6656942	0.9834190	-2.8092948
C	1.8596887	0.2430872	-2.9534737
H	2.5358260	0.1272685	-2.0926667
C	2.1935011	-0.3355185	-4.1852900
H	3.1322872	-0.9012306	-4.2862168
C	1.3285878	-0.2003261	-5.2862262
H	1.5885298	-0.6568313	-6.2532079
C	0.1364762	0.5287414	-5.1469251
H	-0.5405965	0.6483360	-6.0065721
C	-0.1924937	1.1228670	-3.9166867
H	-1.1201144	1.7055691	-3.8191967

S3

75

SCF Energy = -4548.357596040

C	-0.4302162	-2.8888102	-1.9654395
C	-1.3280007	-1.9070489	-1.4918475
C	-1.7980712	-0.9417453	-2.4200299
C	-1.3920745	-0.9630617	-3.7591707
C	-0.5135036	-1.9595699	-4.2145031
C	-0.0350140	-2.9181312	-3.3101258
C	-1.8108727	-1.8689581	-0.0890982
C	-1.1271513	-2.1092980	1.1309798
C	0.2495756	-2.5618266	1.4629380
C	0.7471463	-3.8216529	1.0637167

C	2.0029366	-4.2677676	1.5044245
C	2.7762717	-3.4700062	2.3651465
C	2.2645675	-2.2414676	2.8170306
C	1.0052946	-1.8042093	2.3851278
Br	-1.6490119	2.4396231	1.3649457
C	-3.3400666	-1.6590348	0.2669256
C	-4.3406696	-2.1031175	-0.7985324
C	-3.3488209	-0.1659207	0.5951891
C	-3.4708631	-2.4684929	1.5672971
C	-2.1255139	-2.3069729	2.3008439
O	-2.0575924	-1.2928129	3.2888037
H	-1.8532081	-3.2402395	2.8357092
H	-4.3245470	-2.1395813	2.1924338
H	-3.6162578	-3.5406952	1.3166747
H	-3.8715338	0.1251327	1.5246853
H	-3.6484655	0.5006921	-0.2371576
H	-5.3734472	-1.9976241	-0.4084051
H	-4.1803543	-3.1663964	-1.0738649
H	-4.2661290	-1.5013928	-1.7240613
H	-2.0462770	-0.4310949	2.8059373
H	0.1327574	-4.4739056	0.4272214
H	2.3783172	-5.2473850	1.1719398
H	3.7685664	-3.8125132	2.6948041
H	2.8488614	-1.6075976	3.5003972
H	0.5925071	-0.8589956	2.7568610
H	-2.4786620	-0.1509411	-2.0758099
H	-1.7642635	-0.1927516	-4.4511750
H	-0.1943791	-1.9805928	-5.2671097
H	0.6660015	-3.6949920	-3.6474026
H	-0.0400733	-3.6441735	-1.2769972
Pd	-1.2887152	0.1098433	0.6484887
P	1.0070592	0.6174472	-0.0336568
C	0.9466973	2.1980553	-0.9781232
C	1.9778991	3.1524722	-0.9037457
H	2.8344417	2.9836325	-0.2349478
C	1.9078075	4.3245276	-1.6741679
H	2.7131733	5.0713869	-1.6034132
C	0.8149372	4.5456594	-2.5277139
H	0.7614876	5.4664571	-3.1282242
C	-0.2160086	3.5936367	-2.6050655
H	-1.0813158	3.7664458	-3.2625618
C	-0.1554236	2.4296680	-1.8266032
H	-0.9717431	1.6943085	-1.8656745
C	2.2517039	0.9516767	1.2810079
C	3.6284532	0.6976967	1.1196514
H	4.0068938	0.2995323	0.1675401

C	4.5181923	0.9394168	2.1789650
H	5.5909192	0.7312666	2.0466153
C	4.0425292	1.4426665	3.4008518
H	4.7407817	1.6255222	4.2318355
C	2.6723630	1.7174767	3.5569940
H	2.2931407	2.1204374	4.5082057
C	1.7789910	1.4745861	2.5039050
H	0.7044503	1.6913006	2.6196762
C	1.9033427	-0.4756716	-1.2226957
C	1.9573700	-0.1668796	-2.5975116
H	1.4705859	0.7414639	-2.9774713
C	2.6412544	-1.0101143	-3.4865549
H	2.6759219	-0.7521348	-4.5557437
C	3.2762600	-2.1714073	-3.0203019
H	3.8159316	-2.8271896	-3.7204309
C	3.2193073	-2.4881659	-1.6530789
H	3.7122207	-3.3934346	-1.2673875
C	2.5379133	-1.6496426	-0.7610050
H	2.5292752	-1.8956387	0.3061943

S4

75

SCF Energy = -4548.335835518

C	0.7714860	-2.3270620	-0.6252851
C	-0.3133379	-1.9865731	0.2406005
C	-1.5101121	-1.4427953	-0.3460470
C	-1.6030862	-1.3190950	-1.7644313
C	-0.5517627	-1.7214304	-2.5806000
C	0.6421522	-2.2218295	-2.0050641
C	-0.3362302	-2.4865920	1.6386767
C	-0.3780231	-3.7832378	2.0597237
C	-0.3894662	-5.0153923	1.2513269
C	-0.9630874	-5.0588029	-0.0437773
C	-0.9674784	-6.2468216	-0.7862440
C	-0.4036960	-7.4199334	-0.2554322
C	0.1570137	-7.3949609	1.0323203
C	0.1620552	-6.2090420	1.7802108
Br	-0.7949562	2.6219448	1.6445290
C	-0.3543192	-1.4839360	2.7828113
C	1.0698256	-0.9177961	3.0139312
C	-1.3110035	-0.3490763	2.4137987
C	-0.8041994	-2.3756087	3.9748729
C	-0.3855074	-3.8174971	3.5897339
O	0.8800883	-4.2336531	4.1260702
H	-1.1063215	-4.5670469	3.9774488
H	-0.3721026	-2.0732868	4.9487087

H	-1.9094442	-2.3345645	4.0628919
H	-2.3489035	-0.7037873	2.2457937
H	-1.3227639	0.4613196	3.1650348
H	1.7604257	-1.7014277	3.3867931
H	1.0404906	-0.0994232	3.7610018
H	1.4916315	-0.5011057	2.0755308
H	1.5668350	-3.7640334	3.6143182
H	-1.4328806	-4.1596038	-0.4649055
H	-1.4241497	-6.2581746	-1.7877838
H	-0.4082597	-8.3515903	-0.8414434
H	0.5972575	-8.3088738	1.4599714
H	0.6169828	-6.1795805	2.7812064
H	-2.4391690	-1.4216324	0.2398894
H	-2.5424074	-0.9545110	-2.2062934
H	-0.6381140	-1.6496123	-3.6735185
H	1.4643245	-2.5403752	-2.6595055
H	1.6806676	-2.7532568	-0.1772075
Pd	-0.5718995	0.3959539	0.6051786
P	0.5161327	1.6100624	-1.1987000
C	2.0910443	2.4066532	-0.6595985
C	2.5186482	2.2914870	0.6777277
H	1.8813431	1.7691689	1.4047546
C	3.7348242	2.8639106	1.0835018
H	4.0575743	2.7658854	2.1309483
C	4.5309159	3.5612932	0.1612390
H	5.4822147	4.0125236	0.4821722
C	4.1126670	3.6774267	-1.1757453
H	4.7346454	4.2179556	-1.9054011
C	2.9037689	3.0972982	-1.5870390
H	2.5958935	3.1668422	-2.6409353
C	1.0703110	0.9417334	-2.8316590
C	0.3044986	1.0907068	-4.0046137
H	-0.6334700	1.6638594	-3.9763856
C	0.7379710	0.5200185	-5.2128800
H	0.1323404	0.6494522	-6.1229017
C	1.9422194	-0.2007666	-5.2646967
H	2.2838152	-0.6416332	-6.2133514
C	2.7154575	-0.3446995	-4.0992984
H	3.6651068	-0.9005209	-4.1318176
C	2.2803163	0.2164526	-2.8906254
H	2.8881936	0.0963634	-1.9812435
C	-0.6087684	2.9735448	-1.7122158
C	-0.1996097	4.3099579	-1.8687895
H	0.8400625	4.5960370	-1.6568348
C	-1.1271950	5.2862705	-2.2661270
H	-0.8021419	6.3322627	-2.3741147

C	-2.4640530	4.9358848	-2.5148002
H	-3.1881221	5.7050807	-2.8234113
C	-2.8788727	3.6033940	-2.3499123
H	-3.9294949	3.3251575	-2.5228050
C	-1.9582741	2.6289794	-1.9393205
H	-2.2869417	1.5928887	-1.7648113

Optimized Geometries(BXnd(CH-coord))

R3
75
SCF Energy = -4548.345774304

C	-2.8987673	-1.7193821	-0.8959902
C	-1.9338827	-2.6047919	-0.3234747
C	-1.4590397	-3.6656672	-1.1394558
C	-1.8616519	-3.7831378	-2.4700868
C	-2.7663254	-2.8624187	-3.0386043
C	-3.2941039	-1.8446667	-2.2432110
C	-1.4051802	-2.3697537	1.0365676
C	-0.1640583	-2.7014112	1.5115048
C	0.9804988	-3.3302790	0.8173397
C	1.6797014	-4.4047613	1.4211502
C	2.8213850	-4.9500288	0.8095454
C	3.2848270	-4.4324823	-0.4110554
C	2.5928354	-3.3711034	-1.0215471
C	1.4537316	-2.8252080	-0.4177066
Br	-0.0617353	-0.2087948	-2.6281030
C	-2.1607962	-1.4644248	2.0417836
C	-3.6339699	-1.8525687	2.2618645
C	-2.0058665	0.0073719	1.5582838
C	-1.3508151	-1.7110643	3.3423360
C	0.0606607	-2.0703843	2.8885956
O	0.6983703	-2.8909040	3.8597759
H	0.6663964	-1.1389589	2.7316790
H	-1.3871157	-0.8509979	4.0387014
H	-1.7488498	-2.6029418	3.8704258
H	-1.3916713	0.5878730	2.2669179
H	-2.9818047	0.5295080	1.4474289
H	-3.7233111	-2.9317657	2.5031827
H	-4.2741430	-1.6518591	1.3821508
H	-4.0491341	-1.2742306	3.1127967
H	1.6160018	-3.0301843	3.5561424
H	1.2969279	-4.8293048	2.3607760

H	3.3460880	-5.7914380	1.2879314
H	4.1798382	-4.8597104	-0.8888183
H	2.9403704	-2.9509750	-1.9775330
H	0.9281571	-1.9944589	-0.9154663
H	-0.7560104	-4.3932713	-0.7156378
H	-1.4607612	-4.6045266	-3.0831509
H	-3.0596740	-2.9537161	-4.0944521
H	-4.0171471	-1.1273184	-2.6577674
H	-3.4014236	-0.9621313	-0.2771299
Pd	-1.1315482	0.0137715	-0.3368563
P	0.1310399	1.7893956	0.0935788
C	-0.2047588	3.2752751	-0.9298466
C	-0.9305536	3.1657915	-2.1318594
H	-1.2844642	2.1752251	-2.4569629
C	-1.1624415	4.3093528	-2.9125648
H	-1.7290776	4.2180488	-3.8513892
C	-0.6738095	5.5601016	-2.5014716
H	-0.8590026	6.4542325	-3.1161543
C	0.0508753	5.6710735	-1.3019978
H	0.4352203	6.6492294	-0.9752764
C	0.2837360	4.5342055	-0.5141278
H	0.8426552	4.6243785	0.4292966
C	1.8993556	1.3751646	-0.1478042
C	2.3719328	0.1789444	0.4292336
H	1.6746540	-0.4711609	0.9767517
C	3.7105411	-0.2013175	0.2699452
H	4.0615004	-1.1473048	0.7077405
C	4.5828171	0.6072385	-0.4788240
H	5.6315433	0.3039831	-0.6180878
C	4.1106404	1.7934078	-1.0648023
H	4.7877884	2.4193792	-1.6654253
C	2.7711730	2.1818266	-0.9019806
H	2.3998100	3.1004163	-1.3780383
C	0.0489128	2.4707581	1.8001935
C	1.0602991	2.2469116	2.7538855
H	1.9791239	1.7161587	2.4662086
C	0.8994002	2.7088094	4.0714078
H	1.6957938	2.5312298	4.8098261
C	-0.2658238	3.3971011	4.4432804
H	-0.3886201	3.7574044	5.4757373
C	-1.2769509	3.6244244	3.4923404
H	-2.1935273	4.1622792	3.7779941
C	-1.1247741	3.1592289	2.1798613
H	-1.9222041	3.3253293	1.4390557

R4

75

SCF Energy = -4548.344978397

C	0.6208841	-6.5735041	0.9091586
C	-0.0351404	-5.4113952	0.4296741
C	-0.8956761	-5.5495565	-0.6889221
C	-1.0663349	-6.7887116	-1.3185577
C	-0.3886612	-7.9261414	-0.8463223
C	0.4508008	-7.8114479	0.2735980
C	0.1804188	-4.1153359	1.0957386
Pd	-0.3984707	0.1602304	-0.4176745
P	-0.1493317	2.1761903	0.4691023
C	0.0427673	-2.8601668	0.5794890
Br	0.4087863	0.9424962	-2.6781218
C	-0.3346813	-2.4812829	-0.8037631
C	0.5336803	-2.7448262	-1.8939858
C	0.1196054	-2.5047919	-3.2062304
C	-1.1708047	-2.0047563	-3.4698116
C	-2.0416248	-1.7277352	-2.4128093
C	-1.6307127	-1.9441453	-1.0774639
C	0.6696726	-4.0234482	2.5462878
O	0.1135940	-4.9817926	3.4353911
C	0.3667967	-2.5552397	2.9219390
C	0.4237333	-1.7713709	1.5838398
C	-0.5558061	-0.5918404	1.5196140
C	1.8721434	-1.2993124	1.2970312
H	1.7663573	-4.2165447	2.5825520
H	1.0450151	-2.1493670	3.6980899
H	-0.6690087	-2.5233464	3.3236097
H	-1.5981951	-0.9290810	1.7048071
H	-0.3055145	0.1485132	2.3074803
H	2.1652392	-0.4994125	2.0053618
H	1.9617195	-0.8831687	0.2724771
H	2.5918988	-2.1370118	1.3934727
H	-0.8484643	-4.9979199	3.2669944
H	-1.4486336	-4.6775801	-1.0620520
H	-1.7405865	-6.8676220	-2.1850812
H	-0.5237250	-8.8991720	-1.3426459
H	0.9769110	-8.6972108	0.6614867
H	1.2578368	-6.5047059	1.8007873
H	-2.3581859	-1.8492377	-0.2591755
H	-3.0490909	-1.3334253	-2.6100963
H	-1.4842072	-1.8138914	-4.5060354
H	0.8094359	-2.7027126	-4.0393962
H	1.5325787	-3.1532051	-1.6854347
C	-0.2452629	3.6351280	-0.6389234
C	1.5150106	2.2383630	1.2234325

C	-1.3552854	2.6713773	1.7663513
C	-1.1489647	3.8427268	2.5262832
C	-2.1161307	4.2565917	3.4534322
C	-3.3017370	3.5176868	3.6140635
C	-3.5204063	2.3660693	2.8411587
C	-2.5498558	1.9430581	1.9193006
H	-0.2348496	4.4387867	2.3845715
H	-1.9478136	5.1671639	4.0480680
H	-4.0610692	3.8476050	4.3391542
H	-4.4524905	1.7923515	2.9551250
H	-2.7070251	1.0472431	1.3004363
C	0.6472877	4.7160503	-0.5169197
C	0.4764955	5.8558110	-1.3210677
C	-0.5856545	5.9204223	-2.2358398
C	-1.4794700	4.8404964	-2.3523841
C	-1.3085543	3.6973946	-1.5619729
H	1.4838115	4.6651052	0.1954052
H	1.1822522	6.6955479	-1.2316694
H	-0.7154248	6.8128750	-2.8666610
H	-2.3058162	4.8830264	-3.0775606
H	-1.9833767	2.8357621	-1.6715102
C	1.7254989	2.2319038	2.6158666
C	3.0310586	2.1249567	3.1248915
C	4.1240602	2.0251805	2.2499634
C	3.9125135	2.0277191	0.8587485
C	2.6145059	2.1251807	0.3419900
H	0.8714309	2.2988273	3.3051158
H	3.1913205	2.1154929	4.2135972
H	5.1448159	1.9379877	2.6518904
H	4.7658245	1.9372957	0.1699282
H	2.4347422	2.0782989	-0.7452863

S3

75

SCF Energy = -4548.350703175

C	-2.6152754	-1.5115865	-2.1943885
C	-1.3697556	-1.0480122	-2.7309144
C	-1.4411933	-0.0075796	-3.6986017
C	-2.6494573	0.6153744	-4.0052686
C	-3.8530321	0.2105469	-3.3905609
C	-3.8329373	-0.8737844	-2.5140134
C	-0.0757493	-1.6028639	-2.2760932
C	1.1750528	-1.0785358	-2.4842968
C	1.5931348	0.2595172	-2.9386432
C	0.9639681	1.4221632	-2.4295871
C	1.4416468	2.6943013	-2.7601606

C	2.5675656	2.8419118	-3.5903617
C	3.2120233	1.6995470	-4.0926411
C	2.7319976	0.4193247	-3.7678496
Br	-2.1816252	1.7180861	-0.3357692
C	-0.0090273	-2.8846086	-1.4030524
C	-0.4330955	-4.1374496	-2.1994775
C	-0.8584250	-2.6936963	-0.1178605
C	1.4995875	-2.9493630	-1.0252549
C	2.2566740	-2.0418455	-1.9982159
O	3.3446841	-1.4163847	-1.3187573
H	2.6520115	-2.6216329	-2.8725416
H	1.6528387	-2.5196184	-0.0151756
H	1.8837204	-3.9877073	-0.9999547
H	-0.2888184	-3.0053051	0.7746678
H	-1.8077883	-3.2727957	-0.1214546
H	0.2275806	-4.2888721	-3.0785048
H	-1.4728759	-4.0549469	-2.5732216
H	-0.3716260	-5.0423974	-1.5608999
H	3.6513158	-0.6843991	-1.8931099
H	0.0980492	1.3307067	-1.7541782
H	0.9355741	3.5766223	-2.3407343
H	2.9449795	3.8446821	-3.8421810
H	4.0908203	1.8028283	-4.7475334
H	3.2275692	-0.4698696	-4.1904296
H	-0.5239634	0.3234929	-4.1983648
H	-2.6585148	1.4380394	-4.7361382
H	-4.7958533	0.7276283	-3.6202773
H	-4.7638355	-1.2456873	-2.0613820
H	-2.6595741	-2.4295468	-1.5986439
Pd	-1.4350171	-0.6879395	-0.0775692
P	-0.3344428	-0.2086526	1.7896104
C	-1.3820655	0.3893883	3.1742117
C	-2.7445492	0.6802750	2.9760785
H	-3.1749155	0.5744740	1.9688594
C	-3.5248013	1.1306431	4.0536054
H	-4.5894950	1.3581872	3.8941091
C	-2.9499519	1.2943636	5.3239176
H	-3.5643835	1.6483557	6.1658384
C	-1.5881636	1.0043236	5.5225691
H	-1.1343047	1.1310274	6.5171552
C	-0.8047480	0.5479987	4.4532910
H	0.2586190	0.3114817	4.6103694
C	0.8763507	1.1225884	1.4532026
C	1.9398308	0.8709676	0.5617476
H	2.0779449	-0.1120511	0.0871287
C	2.8404403	1.8966407	0.2427920

H	3.6600107	1.6923464	-0.4619917
C	2.6733767	3.1803551	0.7852110
H	3.3726529	3.9872913	0.5187505
C	1.5987152	3.4368605	1.6532652
H	1.4511376	4.4455531	2.0677634
C	0.6994336	2.4138523	1.9891262
H	-0.1511600	2.6219881	2.6528147
C	0.6089732	-1.5537208	2.6204152
C	2.0144071	-1.6124193	2.6652618
H	2.6167036	-0.8076385	2.2226582
C	2.6533775	-2.7013938	3.2832111
H	3.7527800	-2.7373734	3.3115800
C	1.8981719	-3.7327212	3.8611648
H	2.4024509	-4.5839620	4.3429341
C	0.4931681	-3.6747994	3.8233308
H	-0.1063270	-4.4788746	4.2762015
C	-0.1480339	-2.5952139	3.2030196
H	-1.2481005	-2.5528718	3.1675897

S4

75

SCF Energy = -4548.346538392

C	2.7914445	0.5719182	-1.8438432
C	2.4994738	-0.3264515	-0.7867639
C	1.9507915	-1.6063146	-1.1097202
C	1.7456207	-1.9697179	-2.4605132
C	2.0455291	-1.0677361	-3.4845069
C	2.5612740	0.2052989	-3.1721012
C	2.8625481	-0.0038652	0.6148237
C	4.1145657	0.0492565	1.1553137
C	5.4113298	-0.2072856	0.5020099
C	6.5854497	0.4067260	1.0064698
C	7.8325386	0.1722097	0.4102870
C	7.9401532	-0.6834073	-0.6983343
C	6.7859650	-1.3073743	-1.2025474
C	5.5372745	-1.0745443	-0.6117277
Br	-0.9072841	0.4914505	-2.6577459
C	1.7667596	0.3559065	1.6193671
C	1.2806492	1.8054346	1.3654192
C	0.5906504	-0.6272931	1.5137673
C	2.5366382	0.2539313	2.9662496
C	4.0248526	0.4883801	2.6171182
O	4.4682921	1.8420021	2.8037207
H	4.6954888	-0.1113382	3.2672556
H	2.1823112	0.9703390	3.7332419
H	2.4197518	-0.7714521	3.3741310

H	0.9311923	-1.6739916	1.6647987
H	-0.1544559	-0.4061009	2.3057041
H	2.1011770	2.5347961	1.5214529
H	0.4584457	2.0641495	2.0610306
H	0.8955391	1.9308125	0.3324463
H	4.0994849	2.3602515	2.0624274
H	6.4953304	1.0961916	1.8584335
H	8.7293176	0.6661461	0.8150678
H	8.9194769	-0.8673694	-1.1658111
H	6.8589425	-1.9894729	-2.0634860
H	4.6512399	-1.5885197	-1.0071140
H	1.8402225	-2.3605098	-0.3180325
H	1.3416803	-2.9651153	-2.6957909
H	1.8625935	-1.3435879	-4.5327398
H	2.7805128	0.9190233	-3.9794450
H	3.2119566	1.5573664	-1.5984006
Pd	-0.1519743	-0.4011509	-0.4214500
P	-2.1753627	-0.1839864	0.4577490
C	-2.2471291	1.4541059	1.2666432
C	-2.2481384	1.6175923	2.6654310
H	-2.3170883	0.7406924	3.3251495
C	-2.1455783	2.9054078	3.2186870
H	-2.1412330	3.0288999	4.3121903
C	-2.0434009	4.0274426	2.3815585
H	-1.9599910	5.0341775	2.8181223
C	-2.0390225	3.8628703	0.9839594
H	-1.9472067	4.7390998	0.3247133
C	-2.1315509	2.5828550	0.4232496
H	-2.0783787	2.4398547	-0.6691577
C	-2.6785359	-1.4327267	1.7104015
C	-3.8555200	-1.2527466	2.4683153
H	-4.4519935	-0.3352671	2.3524070
C	-4.2744170	-2.2502070	3.3604115
H	-5.1893295	-2.1025128	3.9538594
C	-3.5347982	-3.4394262	3.4875308
H	-3.8683958	-4.2222570	4.1854279
C	-2.3775323	-3.6313853	2.7160126
H	-1.8032091	-4.5659399	2.8034984
C	-1.9495239	-2.6307431	1.8293283
H	-1.0491195	-2.7666022	1.2121188
C	-3.6231442	-0.2442695	-0.6670397
C	-4.7096032	0.6379328	-0.5205836
H	-4.6695560	1.4461461	0.2243922
C	-5.8408365	0.4935897	-1.3416849
H	-6.6848735	1.1914349	-1.2328313
C	-5.8914995	-0.5321382	-2.2980159

H	-6.7772363	-0.6410130	-2.9421008
C	-4.8061700	-1.4157303	-2.4390958
H	-4.8377527	-2.2131982	-3.1964376
C	-3.6714227	-1.2707715	-1.6315561
H	-2.8054916	-1.9368478	-1.7591043

Optimized Geometries(BXn(TS-de))

R3
75
SCF Energy = -4548.298413933

C	-1.1288940	5.0810525	0.2205093
C	-0.9161748	3.6956040	0.0483167
C	-0.9567290	3.1482218	-1.2535840
C	-1.2471107	3.9637749	-2.3553136
C	-1.4958705	5.3353987	-2.1700683
C	-1.4287482	5.8973878	-0.8836968
C	-0.6374732	2.8722162	1.2346631
C	0.4521454	2.0988834	1.4770008
C	1.6513632	1.9924269	0.6252610
C	2.2359545	0.7384522	0.3278968
C	3.4012046	0.6625844	-0.4529358
C	3.9973231	1.8349340	-0.9460991
C	3.4210792	3.0848654	-0.6582766
C	2.2598820	3.1672562	0.1210827
Br	1.3406936	7.0523764	1.0151264
C	-1.5659276	2.9621323	2.4525239
C	-3.0543791	2.8814417	2.0948998
C	-1.2493256	4.2454708	3.2200888
C	-1.0777977	1.7398785	3.2923555
C	0.3852313	1.5088582	2.8839516
O	0.7006495	0.1228840	2.9912717
H	1.0816029	2.0968117	3.5363146
H	-1.2169542	1.8722443	4.3841191
H	-1.6443593	0.8377794	2.9807663
H	-0.2845429	4.1528370	3.7594067
H	-2.0466573	4.5259119	3.9328682
H	-3.2665238	1.9830748	1.4821418
H	-3.3751914	3.7689747	1.5118342
H	-3.6718777	2.8325056	3.0150980
H	1.6622373	0.0402075	2.8456842
H	1.7430112	-0.1782880	0.6842497
H	3.8403840	-0.3195471	-0.6856388

H	4.9121421	1.7752119	-1.5557223
H	3.8799533	4.0100816	-1.0378318
H	1.8259539	4.1513701	0.3574227
H	-0.7548409	2.0742699	-1.3830942
H	-1.2809545	3.5284372	-3.3658777
H	-1.7307346	5.9776520	-3.0331396
H	-1.5799844	6.9778129	-0.7468830
H	-2.1221693	5.5590083	1.7447602
Pd	-0.6411613	5.8797607	2.0533853
P	-0.1699858	7.0474093	4.0920250
C	-0.4068871	8.8716360	4.0467420
C	-0.3638085	9.5717500	2.8242603
H	-0.1702255	9.0204951	1.8911412
C	-0.5303295	10.9663543	2.8120551
H	-0.4906482	11.5078756	1.8549989
C	-0.7462934	11.6663776	4.0102382
H	-0.8787601	12.7589372	3.9959881
C	-0.7946740	10.9682002	5.2294601
H	-0.9691964	11.5094931	6.1716821
C	-0.6269334	9.5765484	5.2508090
H	-0.6723471	9.0342406	6.2066753
C	1.5607768	6.7939196	4.6299284
C	1.9815287	5.4958042	4.9939271
H	1.2540913	4.6707224	5.0424430
C	3.3279458	5.2500618	5.2969857
H	3.6474384	4.2366846	5.5820876
C	4.2668827	6.2936990	5.2260738
H	5.3243264	6.0978951	5.4584200
C	3.8533691	7.5822373	4.8532316
H	4.5872361	8.3992675	4.7870503
C	2.5056309	7.8351060	4.5531240
H	2.1875181	8.8412990	4.2460939
C	-1.2054477	6.5806621	5.5378570
C	-0.6860538	6.2948276	6.8150254
H	0.4005377	6.3174569	6.9826794
C	-1.5569057	5.9949814	7.8768944
H	-1.1453193	5.7786649	8.8743354
C	-2.9453090	5.9808532	7.6718186
H	-3.6240458	5.7467399	8.5056677
C	-3.4680560	6.2678338	6.3979817
H	-4.5556111	6.2592378	6.2314312
C	-2.6033170	6.5625474	5.3357488
H	-3.0093863	6.7858024	4.3359525

R4
75

SCF Energy = -4548.295973134

C	2.9035519	-0.1395570	0.8163669
C	1.7050964	0.4935919	0.4088194
C	0.7489788	-0.2752795	-0.3000344
C	0.9992583	-1.6137634	-0.6234196
C	2.2076830	-2.2218367	-0.2368331
C	3.1546170	-1.4800350	0.4876731
C	1.4218574	1.8895475	0.7862797
Pd	-1.3923043	5.2865331	-0.9245534
P	-2.4643239	7.0862755	0.2374659
C	0.8081500	2.8841695	0.0685210
Br	-0.8167677	6.9710114	-2.7271372
C	0.5043408	2.9025855	-1.3751589
C	1.2737193	2.1003225	-2.2614925
C	0.9888474	2.0295041	-3.6266950
C	-0.0782803	2.7750602	-4.1564241
C	-0.8054967	3.6314384	-3.3175120
C	-0.4960914	3.7364140	-1.9461942
C	1.7994971	2.3830033	2.1831966
O	1.7483484	1.4065756	3.2107260
C	0.8444324	3.5769873	2.3848627
C	0.5057564	4.0980701	0.9551477
C	-0.9875536	4.4255547	0.9212949
C	1.3944756	5.3087415	0.5926956
H	2.8594301	2.7291851	2.1807704
H	1.2508647	4.3721900	3.0395279
H	-0.0689042	3.1770981	2.8753616
H	-1.5863501	3.5197056	1.1306050
H	-1.2432837	5.1939749	1.6770039
H	1.1538409	6.1788046	1.2352379
H	1.2602104	5.6155126	-0.4640262
H	2.4643885	5.0563516	0.7354354
H	0.9428653	0.8757922	3.0563973
H	-0.1982824	0.1978434	-0.5980193
H	0.2432680	-2.1911491	-1.1772899
H	2.4043627	-3.2745251	-0.4906270
H	4.0978276	-1.9505551	0.8049048
H	3.6455907	0.4281657	1.3951088
H	-2.1248014	3.9396653	-0.8903744
H	-1.5959428	4.2642293	-3.7447843
H	-0.3234280	2.7207989	-5.2282209
H	1.6049082	1.3938390	-4.2805108
H	2.1175338	1.5270508	-1.8549835
C	-3.3100947	8.3969786	-0.7208957
C	-1.1657212	7.9349679	1.2115027
C	-3.7515972	6.6077240	1.4630461

C	-4.3096245	7.5622071	2.3408947
C	-5.3202348	7.1874293	3.2370741
C	-5.7896753	5.8615370	3.2573045
C	-5.2488936	4.9128470	2.3754498
C	-4.2328441	5.2847290	1.4799090
H	-3.9539441	8.6033312	2.3189159
H	-5.7493941	7.9355002	3.9206791
H	-6.5849038	5.5705570	3.9602040
H	-5.6197871	3.8768631	2.3814352
H	-3.8082713	4.5509460	0.7787404
C	-3.2595057	9.7531148	-0.3455582
C	-3.9840533	10.7081070	-1.0772532
C	-4.7615565	10.3122639	-2.1773299
C	-4.8117307	8.9580567	-2.5518012
C	-4.0838362	8.0020472	-1.8310538
H	-2.6418348	10.0662063	0.5093254
H	-3.9365776	11.7684667	-0.7863894
H	-5.3254676	11.0631182	-2.7512383
H	-5.4097803	8.6467876	-3.4212698
H	-4.0955802	6.9457079	-2.1384489
C	-1.0104792	7.7170591	2.5963152
C	0.1059676	8.2404055	3.2699523
C	1.0675316	8.9855140	2.5695254
C	0.9141449	9.2043003	1.1886393
C	-0.1900064	8.6760961	0.5063055
H	-1.7618587	7.1372289	3.1519345
H	0.2218737	8.0625423	4.3497003
H	1.9419444	9.3931585	3.0988658
H	1.6700126	9.7790215	0.6327428
H	-0.2864142	8.8014284	-0.5837034

S3

75

SCF Energy = -4548.301392910

C	-1.2638786	4.7790970	0.2680791
C	-1.3040587	3.3704567	0.0807666
C	-1.6916152	2.8317204	-1.1574710
C	-2.0429185	3.6876460	-2.2152524
C	-1.9767470	5.0790401	-2.0428088
C	-1.5858518	5.6262453	-0.8054532
C	-0.6912567	2.6212546	1.1992169
C	0.6301772	2.2924131	1.2629940
C	1.6539365	2.3063001	0.1946858
C	1.7037874	3.3104827	-0.8015606
C	2.7169510	3.2985885	-1.7708142
C	3.6936330	2.2894611	-1.7716583

C	3.6617567	1.2919203	-0.7821838
C	2.6569890	1.3066728	0.1949929
Br	1.4790486	6.5588676	1.0456168
C	-1.3768018	2.5921213	2.5787862
C	-2.5838644	1.6310035	2.5639066
C	-1.8557162	4.0027658	2.9557045
C	-0.2307816	2.0760204	3.4995963
C	1.0544781	2.3303687	2.7192220
O	1.4501437	3.7136278	2.9750519
H	1.8991012	1.6653083	2.9992668
H	-0.2130597	2.5781808	4.4869127
H	-0.3386372	0.9862129	3.6705162
H	-1.9015021	4.1394678	4.0502109
H	-2.8491227	4.2180304	2.5192157
H	-2.2659712	0.6015279	2.2988479
H	-3.3373254	1.9626373	1.8211428
H	-3.0719136	1.6011259	3.5601753
H	1.9830594	4.0503417	2.2159651
H	0.9732388	4.1280611	-0.7922420
H	2.7473707	4.0994295	-2.5247774
H	4.4855800	2.2848770	-2.5361013
H	4.4252263	0.4990311	-0.7706264
H	2.6333228	0.5205025	0.9657692
H	-1.6730556	1.7405019	-1.2993748
H	-2.3443063	3.2651654	-3.1856750
H	-2.2273979	5.7512721	-2.8778555
H	-1.5095286	6.7172796	-0.6875845
H	-1.7400504	5.8587915	1.5264784
Pd	-0.4539068	5.3177034	2.1475423
P	0.0073303	6.4634036	4.2016433
C	-0.9041635	8.0610220	4.1753063
C	-1.0438450	8.7261774	2.9388467
H	-0.6277832	8.2653494	2.0288698
C	-1.6818162	9.9747000	2.8816004
H	-1.7836178	10.4884514	1.9137466
C	-2.1880572	10.5653250	4.0515658
H	-2.6941629	11.5415169	4.0028252
C	-2.0428999	9.9095366	5.2857915
H	-2.4302131	10.3717047	6.2065698
C	-1.3979680	8.6645030	5.3511419
H	-1.2754242	8.1601256	6.3208587
C	1.7299596	6.9688529	4.6075996
C	2.7617900	6.0065099	4.5603841
H	2.5286862	4.9755243	4.2575524
C	4.0779178	6.3726071	4.8773802
H	4.8756929	5.6153541	4.8374506

C	4.3818830	7.6996447	5.2236807
H	5.4178382	7.9863546	5.4602296
C	3.3600839	8.6614977	5.2543115
H	3.5908700	9.7059398	5.5136472
C	2.0381946	8.3007049	4.9494628
H	1.2472872	9.0632415	4.9694769
C	-0.5976498	5.6259546	5.7220048
C	0.2793968	4.9442955	6.5895911
H	1.3653786	5.0104761	6.4328508
C	-0.2276443	4.1897478	7.6598908
H	0.4692366	3.6661353	8.3318143
C	-1.6124178	4.1087501	7.8789987
H	-2.0062560	3.5186916	8.7201855
C	-2.4928382	4.7879919	7.0199579
H	-3.5796059	4.7330693	7.1845811
C	-1.9916068	5.5345937	5.9434751
H	-2.6878582	6.0606569	5.2726188

S4

75

SCF Energy = -4548.299601431

C	1.3763977	3.8864895	-1.7935601
C	0.5437194	3.9853846	-0.6460929
C	-0.6784753	4.7000402	-0.7733934
C	-1.0983128	5.1551904	-2.0400844
C	-0.2865041	4.9866905	-3.1709043
C	0.9716233	4.3740746	-3.0379181
C	0.9922637	3.3895395	0.6255530
C	1.8282084	2.3132431	0.7949425
C	2.3188268	1.3392835	-0.1983990
C	3.6460091	0.8512224	-0.1331456
C	4.1000708	-0.1101570	-1.0489831
C	3.2379759	-0.6103430	-2.0382088
C	1.9105819	-0.1480230	-2.0994895
C	1.4546222	0.8129566	-1.1893985
Br	-1.8708252	7.7083225	0.0428173
C	0.5441301	3.9686522	1.9706381
C	1.0581121	5.4072280	2.1987800
C	-0.9774973	3.8617026	2.0907327
C	1.1699788	2.9773623	3.0049357
C	2.2689702	2.2093639	2.2475918
O	3.5885757	2.7526370	2.4230849
H	2.3530427	1.1588262	2.5937474
H	1.5722908	3.4967600	3.8964170
H	0.4041688	2.2549044	3.3561707
H	-1.3126582	2.8323086	1.8651667

H	-1.3153432	4.1265169	3.1113728
H	2.1661304	5.4178333	2.2360281
H	0.6829041	5.8081984	3.1612514
H	0.7388623	6.0968844	1.3918382
H	3.6168627	3.5695476	1.8867401
H	4.3152216	1.2508736	0.6431131
H	5.1383336	-0.4711837	-0.9884325
H	3.5952000	-1.3643071	-2.7560631
H	1.2228213	-0.5460026	-2.8613499
H	0.4143139	1.1670507	-1.2343759
H	-2.1831085	3.9444924	0.2513381
H	-2.0542721	5.6887936	-2.1353031
H	-0.6250750	5.3645875	-4.1478530
H	1.6405328	4.2783979	-3.9064760
H	2.3635604	3.4158323	-1.6894920
Pd	-1.8027552	5.3076956	0.8434493
P	-3.1464321	6.0223266	2.6950168
C	-1.9901776	6.6613631	3.9645128
C	-1.6240408	5.8965766	5.0915383
H	-2.1401958	4.9498397	5.3076185
C	-0.5984627	6.3432499	5.9418576
H	-0.3159325	5.7386954	6.8168369
C	0.0610409	7.5537168	5.6769142
H	0.8646425	7.9009804	6.3436645
C	-0.3040332	8.3187050	4.5545360
H	0.2157047	9.2638135	4.3369508
C	-1.3171788	7.8748267	3.6941097
H	-1.5703541	8.4453948	2.7867541
C	-4.1185723	4.7125106	3.5476799
C	-4.7929607	4.9816667	4.7584707
H	-4.7219916	5.9793817	5.2172519
C	-5.5558029	3.9807729	5.3758672
H	-6.0762162	4.1954550	6.3214668
C	-5.6607092	2.7081086	4.7858525
H	-6.2615500	1.9246786	5.2720346
C	-5.0058900	2.4411923	3.5733779
H	-5.0933372	1.4501625	3.1032675
C	-4.2371513	3.4409010	2.9551611
H	-3.7269669	3.2444540	2.0005614
C	-4.3945087	7.3382299	2.4453046
C	-4.6323670	8.3403963	3.4053945
H	-4.0152053	8.3912629	4.3147554
C	-5.6464205	9.2877503	3.1898448
H	-5.8248514	10.0746991	3.9382425
C	-6.4248786	9.2343334	2.0226149
H	-7.2159867	9.9806117	1.8541852

C	-6.1868129	8.2337552	1.0641729
H	-6.7864254	8.1974501	0.1423886
C	-5.1710321	7.2908859	1.2698132
H	-4.9605892	6.5248974	0.5085248

Optimized Geometries(BXne)

R3
75
SCF Energy = -4548.305156062

C	-1.8169781	0.1299533	-0.4239995
C	-1.5902119	0.3858594	-1.7961403
C	-2.0420486	1.6306276	-2.3066073
C	-2.7207475	2.5477618	-1.4983419
C	-2.9898558	2.2346128	-0.1562425
C	-2.5437562	1.0170358	0.3824322
C	-0.9877532	-0.6167852	-2.6837770
C	-0.1231040	-0.4353638	-3.7223059
C	0.5854724	0.7954885	-4.1092287
C	0.7383047	1.1515492	-5.4702689
C	1.4385212	2.3139993	-5.8272147
C	2.0124406	3.1296140	-4.8376585
C	1.8912755	2.7670756	-3.4840343
C	1.1842753	1.6134592	-3.1227994
Br	1.6587599	-1.3867512	-0.6133451
C	-1.4569449	-2.0776777	-2.5597247
C	-2.9089223	-2.1738653	-3.0876810
C	-1.4196809	-2.6058434	-1.1161220
C	-0.4428181	-2.7977613	-3.4936389
C	0.0544797	-1.7355748	-4.4950303
O	-0.6565505	-1.7038383	-5.7462244
H	1.1114613	-1.9049108	-4.7841462
H	0.4224480	-3.1243773	-2.8832833
H	-0.8684475	-3.6817243	-4.0089709
H	-0.6725649	-3.4136534	-0.9821739
H	-2.4120855	-2.9515897	-0.7754131
H	-2.9848557	-1.8278700	-4.1390728
H	-3.5902124	-1.5466806	-2.4775559
H	-3.2708356	-3.2216092	-3.0495731
H	-1.5517610	-1.3689761	-5.5436314
H	0.2950862	0.4992127	-6.2370668
H	1.5413997	2.5825340	-6.8899520
H	2.5677006	4.0369575	-5.1205051

H	2.3732518	3.3790521	-2.7055437
H	1.1151330	1.2979957	-2.0738376
H	-1.8553572	1.8529730	-3.3672085
H	-3.0577766	3.5051661	-1.9226230
H	-3.5353487	2.9403147	0.4876145
H	-2.7285313	0.7960447	1.4415553
H	-2.0211002	-1.5660241	1.0833747
Pd	-0.6790619	-1.3254496	0.3614448
P	0.2026479	-0.0423375	2.2482297
C	0.0985934	1.7378462	1.8206620
C	0.5917296	2.1221576	0.5545252
H	1.1012422	1.3714544	-0.0704390
C	0.3995714	3.4301532	0.0953394
H	0.7555099	3.7120294	-0.9060644
C	-0.2756333	4.3668935	0.8981940
H	-0.4382953	5.3908303	0.5293519
C	-0.7492674	3.9925033	2.1650252
H	-1.2757183	4.7239370	2.7969053
C	-0.5691144	2.6780514	2.6275449
H	-0.9653772	2.3803718	3.6091875
C	1.9507301	-0.3252668	2.7112652
C	2.3629646	-1.6547380	2.9387920
H	1.6473238	-2.4808041	2.8064191
C	3.6849702	-1.9246043	3.3140867
H	4.0027536	-2.9638161	3.4863242
C	4.6076559	-0.8719128	3.4494152
H	5.6491816	-1.0864748	3.7327360
C	4.2021305	0.4508031	3.2126478
H	4.9234192	1.2761738	3.3109393
C	2.8746344	0.7278324	2.8455342
H	2.5566414	1.7633588	2.6550505
C	-0.6800201	-0.1705214	3.8570266
C	-0.0543173	0.2182019	5.0613417
H	0.9900044	0.5645872	5.0462937
C	-0.7604091	0.1583563	6.2721302
H	-0.2656983	0.4613866	7.2073668
C	-2.0925756	-0.2903043	6.2926682
H	-2.6427882	-0.3388045	7.2445437
C	-2.7164119	-0.6875116	5.0986973
H	-3.7547966	-1.0514329	5.1106536
C	-2.0106410	-0.6329934	3.8864910
H	-2.4857714	-0.9675673	2.9498906

R3(TS-eX)

75

SCF Energy = -4548.293869515

C	-1.3469473	-1.1019616	-0.6612764
C	-1.2669476	-2.4939673	-0.4735918
C	-1.7042685	-3.3242797	-1.5381873
C	-2.1952841	-2.7794152	-2.7287663
C	-2.2792563	-1.3847333	-2.8814048
C	-1.8586987	-0.5394093	-1.8394624
C	-0.8378605	-3.0613446	0.8069598
C	-0.1501031	-4.2141185	1.0548703
C	0.5605384	-5.0584986	0.0803807
C	0.5636063	-6.4686253	0.1984542
C	1.2663184	-7.2568926	-0.7252703
C	1.9825955	-6.6520986	-1.7717176
C	2.0030897	-5.2497448	-1.8824215
C	1.3029373	-4.4561926	-0.9653710
Br	1.8644344	-0.4352059	-0.2663505
C	-1.2377807	-2.3171703	2.0804220
C	-2.7640541	-2.1553879	2.2006960
C	-0.5248855	-0.9787316	2.1117096
C	-0.6392792	-3.2333420	3.2075657
C	-0.2237012	-4.5625853	2.5322331
O	-1.1544771	-5.6350450	2.7561787
H	0.7387729	-4.9446583	2.9295231
H	0.2496624	-2.7559894	3.6670405
H	-1.3671084	-3.4215568	4.0209527
H	0.5709153	-1.1042560	2.1894451
H	-0.9238935	-0.2930808	2.8865879
H	-3.2659878	-3.1438671	2.2168602
H	-3.1689315	-1.5784382	1.3462651
H	-3.0276924	-1.6219117	3.1368373
H	-1.9364458	-5.4297240	2.2061965
H	-0.0048670	-6.9300567	1.0195281
H	1.2540114	-8.3533952	-0.6267643
H	2.5343510	-7.2722246	-2.4948405
H	2.5814480	-4.7677549	-2.6855185
H	1.3459865	-3.3574803	-1.0295987
H	-1.6516443	-4.4148174	-1.4060475
H	-2.5267899	-3.4462244	-3.5387044
H	-2.6774065	-0.9415786	-3.8068275
H	-1.9218114	0.5514633	-1.9654196
H	-1.8994736	0.7272085	0.9051969
Pd	-0.4666717	0.3002606	0.4696958
P	0.0952430	2.6489965	-0.0421157
C	-0.2855598	2.7572942	-1.8384928
C	0.4454276	1.9291837	-2.7208301
H	1.2470044	1.2836572	-2.3252833
C	0.1140972	1.8993240	-4.0816222

H	0.6818755	1.2466803	-4.7615718
C	-0.9491042	2.6789938	-4.5715007
H	-1.2133151	2.6436765	-5.6392894
C	-1.6752254	3.5011018	-3.6945473
H	-2.5056807	4.1163054	-4.0730101
C	-1.3453292	3.5455909	-2.3295078
H	-1.9159540	4.1906420	-1.6455753
C	1.8300669	3.2082175	0.1000661
C	2.5722813	2.7924029	1.2237490
H	2.1168162	2.1068734	1.9540327
C	3.8930766	3.2308242	1.3921436
H	4.4712790	2.8988340	2.2673012
C	4.4832710	4.0721276	0.4334622
H	5.5242409	4.4057324	0.5611260
C	3.7503209	4.4762582	-0.6948067
H	4.2140881	5.1273783	-1.4512155
C	2.4247361	4.0461537	-0.8644853
H	1.8519282	4.3525460	-1.7525925
C	-0.8986106	3.9990003	0.7092362
C	-0.3910570	5.3076936	0.8485298
H	0.6377873	5.5334248	0.5317762
C	-1.1973263	6.3185335	1.3945444
H	-0.7934835	7.3363602	1.5050640
C	-2.5128277	6.0345413	1.7983553
H	-3.1417252	6.8297451	2.2264921
C	-3.0207151	4.7312671	1.6638108
H	-4.0474160	4.5011575	1.9862308
C	-2.2141475	3.7146646	1.1305101
H	-2.5964069	2.6847319	1.0411614

R3X

75

SCF Energy = -4548.305137061

C	-1.2244911	-0.4910931	1.4333816
C	-1.2440629	-1.8453310	1.0269840
C	-2.4494141	-2.3341932	0.4593230
C	-3.5836040	-1.5244240	0.3457499
C	-3.5523692	-0.2035042	0.8211137
C	-2.3705412	0.3142086	1.3749939
C	-0.1019675	-2.7402539	1.2518826
C	0.3727116	-3.7422640	0.4583545
C	-0.0161295	-4.0667252	-0.9238662
C	-0.1681883	-5.4099040	-1.3424843
C	-0.5143831	-5.7065313	-2.6695722
C	-0.6967272	-4.6733953	-3.6040695
C	-0.5178549	-3.3368649	-3.2039597

C	-0.1826355	-3.0358737	-1.8779866
Br	2.2866267	-0.5971334	-0.0102504
C	0.6181793	-2.6774083	2.6109911
C	-0.3244056	-3.2569821	3.6934814
C	1.0209748	-1.2505368	3.0187194
C	1.8427411	-3.5983243	2.3433618
C	1.4296089	-4.5486443	1.2012150
O	0.9121586	-5.8214081	1.6307047
H	2.2883941	-4.8072495	0.5492271
H	2.6792465	-2.9694058	1.9795559
H	2.1803716	-4.1552504	3.2400461
H	2.1207302	-1.1152209	3.0471281
H	0.5807586	-0.9565248	3.9883694
H	-0.6247699	-4.2988002	3.4584100
H	-1.2494919	-2.6506112	3.7731984
H	0.1747782	-3.2643497	4.6838538
H	0.0477114	-5.6383972	2.0476403
H	-0.0111764	-6.2110505	-0.6052916
H	-0.6377914	-6.7561469	-2.9781048
H	-0.9608774	-4.9089991	-4.6463232
H	-0.6186081	-2.5241460	-3.9403082
H	-0.0015499	-2.0006467	-1.5614930
H	-2.4744529	-3.3798363	0.1198849
H	-4.5032521	-1.9316623	-0.0999313
H	-4.4413541	0.4406683	0.7513032
H	-2.3451675	1.3585943	1.7115954
H	-0.1559064	0.9532203	2.8334964
Pd	0.6092074	0.2913757	1.6685057
P	0.2934343	2.2453315	0.2317361
C	-1.0537362	1.8653376	-0.9531385
C	-0.9812498	0.6281418	-1.6299685
H	-0.0865645	-0.0008865	-1.4981450
C	-2.0505213	0.2007676	-2.4253774
H	-2.0009036	-0.7795435	-2.9207578
C	-3.1946427	1.0073827	-2.5603774
H	-4.0403538	0.6633456	-3.1746906
C	-3.2607252	2.2461298	-1.9041935
H	-4.1537384	2.8808175	-2.0098770
C	-2.1952309	2.6761810	-1.0955758
H	-2.2617706	3.6348220	-0.5608958
C	1.7118471	2.7648302	-0.8018740
C	2.9488294	2.9794364	-0.1592744
H	3.0414716	2.8045828	0.9237518
C	4.0612970	3.3965253	-0.9007245
H	5.0251069	3.5588346	-0.3954071
C	3.9508404	3.5869043	-2.2897606

H	4.8286826	3.9034230	-2.8730999
C	2.7234812	3.3629512	-2.9327721
H	2.6354398	3.5043746	-4.0206319
C	1.6019694	2.9539680	-2.1920590
H	0.6407795	2.7737290	-2.6953546
C	-0.2380969	3.8164003	1.0274878
C	-0.0854767	5.0534597	0.3646242
H	0.3959030	5.0864314	-0.6242770
C	-0.5421437	6.2353461	0.9668966
H	-0.4185179	7.1963164	0.4448712
C	-1.1516456	6.1942404	2.2330563
H	-1.5065768	7.1234646	2.7039203
C	-1.2965510	4.9673665	2.9011337
H	-1.7613660	4.9308851	3.8978589
C	-0.8363335	3.7838889	2.3027134
H	-0.9239220	2.8215109	2.8329019

R4

75

SCF Energy = -4548.298276561

C	-0.3263803	-6.5809788	1.1589195
C	-0.7665213	-5.3170139	0.6977858
C	-1.9906128	-5.2530006	-0.0133887
C	-2.7257049	-6.4124539	-0.2857256
C	-2.2619310	-7.6654521	0.1552708
C	-1.0626686	-7.7424359	0.8817211
C	-0.0154644	-4.0914565	1.0207993
Pd	-0.0333349	0.3108517	-0.8185620
P	-0.0056722	2.5514624	0.1105219
C	0.2016656	-2.9736521	0.2580190
Br	2.0711258	0.9099301	-2.0992836
C	-0.0215654	-2.7804811	-1.1844927
C	-0.0260040	-3.9006427	-2.0605446
C	-0.2580915	-3.7595188	-3.4299920
C	-0.4828277	-2.4817644	-3.9714189
C	-0.4259824	-1.3566934	-3.1342721
C	-0.1735089	-1.4926617	-1.7553850
C	0.6310087	-3.9397045	2.3966780
O	-0.0578170	-4.5642610	3.4676790
C	0.7735455	-2.4082359	2.5384232
C	0.8503585	-1.8546946	1.0776907
C	0.0016218	-0.5928028	1.0502457
C	2.3148186	-1.6186155	0.6602623
H	1.6367772	-4.4208308	2.3926308
H	1.6379517	-2.0928870	3.1537770
H	-0.1457996	-2.0490377	3.0478845

H	-1.0243186	-0.8139339	1.3949784
H	0.4431398	0.2187927	1.6622222
H	2.7560747	-0.7879477	1.2481252
H	2.3951849	-1.3523282	-0.4108832
H	2.9152142	-2.5328455	0.8388931
H	-1.0113102	-4.4168905	3.3142335
H	-2.3570910	-4.2733266	-0.3535565
H	-3.6726465	-6.3389587	-0.8421406
H	-2.8404665	-8.5770709	-0.0580290
H	-0.6972455	-8.7167540	1.2406977
H	0.6039036	-6.6512467	1.7397799
H	-1.5132232	0.0769397	-0.4789370
H	-0.5435357	-0.3553962	-3.5773040
H	-0.6662898	-2.3535425	-5.0493725
H	-0.2524651	-4.6471977	-4.0803331
H	0.1684707	-4.8980957	-1.6435926
C	0.5033041	3.8962308	-1.0196011
C	1.1758020	2.6264398	1.5155569
C	-1.5800696	3.1684088	0.8361126
C	-1.8718275	4.5471286	0.8994521
C	-3.0626449	4.9877078	1.4973367
C	-3.9678449	4.0595171	2.0391403
C	-3.6830133	2.6852394	1.9759047
C	-2.4974729	2.2407246	1.3710636
H	-1.1650938	5.2753893	0.4749126
H	-3.2855562	6.0646720	1.5382429
H	-4.9015527	4.4079771	2.5059024
H	-4.3920113	1.9533004	2.3911627
H	-2.2807791	1.1642676	1.3060976
C	1.3734141	4.9278844	-0.6185692
C	1.7057197	5.9521147	-1.5204951
C	1.1693457	5.9511769	-2.8180228
C	0.3007192	4.9207771	-3.2190178
C	-0.0269847	3.8922147	-2.3261178
H	1.7974016	4.9243610	0.3963325
H	2.3912327	6.7537013	-1.2063418
H	1.4351962	6.7522811	-3.5241553
H	-0.1110901	4.9104237	-4.2392222
H	-0.6850632	3.0699898	-2.6464895
C	0.7639791	2.9483423	2.8245779
C	1.6878816	2.9005250	3.8820557
C	3.0215790	2.5356584	3.6392578
C	3.4335936	2.2164229	2.3328970
C	2.5176889	2.2536407	1.2724988
H	-0.2798890	3.2346090	3.0187615
H	1.3599354	3.1511157	4.9022832

H	3.7422280	2.4970540	4.4701584
H	4.4770237	1.9267080	2.1368958
H	2.8264763	1.9780114	0.2502628

S3

75

SCF Energy = -4548.305956452

C	-1.5632412	-1.7695660	-1.3238376
C	-1.8702445	-2.8655888	-0.4786208
C	-2.4429384	-4.0373307	-0.9994339
C	-2.7164222	-4.1219174	-2.3753212
C	-2.4022815	-3.0445572	-3.2192364
C	-1.8267241	-1.8680328	-2.6982313
C	-1.3763590	-2.6344911	0.8948526
C	-0.1164351	-2.9383754	1.3165000
C	0.8921777	-3.8334587	0.7070912
C	1.0689957	-3.9441069	-0.6929608
C	2.0699058	-4.7743432	-1.2175740
C	2.9076818	-5.5110969	-0.3646605
C	2.7488142	-5.4033924	1.0275329
C	1.7566995	-4.5663252	1.5561744
Br	1.4114961	-0.3314527	-1.8681285
C	-2.0377154	-1.5314565	1.7447253
C	-3.3706262	-2.0290236	2.3412211
C	-2.3112243	-0.2915899	0.8749581
C	-0.9619200	-1.2771219	2.8422225
C	0.3275817	-1.8348889	2.2536626
O	0.8710493	-0.7969779	1.3678542
H	1.1082778	-2.0941472	2.9986050
H	-0.8612196	-0.2067736	3.1100837
H	-1.2088291	-1.8401761	3.7642837
H	-2.3846435	0.6235984	1.4897827
H	-3.2360873	-0.4153757	0.2825993
H	-3.2074369	-2.9183107	2.9843683
H	-4.0767119	-2.3103213	1.5341113
H	-3.8457252	-1.2354077	2.9545839
H	1.4786050	-1.2028047	0.7012030
H	0.4461954	-3.3489132	-1.3716661
H	2.2017394	-4.8323738	-2.3084321
H	3.6905972	-6.1619745	-0.7829928
H	3.4026692	-5.9736141	1.7050855
H	1.6323455	-4.4884715	2.6477676
H	-2.6423144	-4.8880339	-0.3301348
H	-3.1617053	-5.0381798	-2.7917042
H	-2.6018923	-3.1161454	-4.2998998
H	-1.5587814	-1.0440287	-3.3754270

H	-1.7034775	0.5187433	-1.3429188
Pd	-0.6936955	-0.1142474	-0.4221539
P	0.0523508	2.1027836	0.2463914
C	-0.5642174	3.3231897	-0.9824588
C	-0.5463003	2.9512797	-2.3442711
H	-0.1892078	1.9479098	-2.6272818
C	-0.9533337	3.8667005	-3.3267036
H	-0.9336059	3.5699861	-4.3861766
C	-1.3837977	5.1531843	-2.9607643
H	-1.7095324	5.8667694	-3.7328229
C	-1.3926798	5.5294727	-1.6071267
H	-1.7205657	6.5390182	-1.3160131
C	-0.9777850	4.6218003	-0.6197099
H	-0.9730139	4.9251613	0.4374755
C	1.8436424	2.5096475	0.3668093
C	2.7027311	1.6642314	1.1017105
H	2.2945251	0.7586993	1.5710961
C	4.0668064	1.9704452	1.2109359
H	4.7278877	1.3040142	1.7855873
C	4.5913934	3.1083866	0.5761378
H	5.6644217	3.3403198	0.6541916
C	3.7424176	3.9421828	-0.1683935
H	4.1463201	4.8305167	-0.6773400
C	2.3740605	3.6476712	-0.2739363
H	1.7204312	4.3040643	-0.8649775
C	-0.6628686	2.6488154	1.8467224
C	0.0993121	2.6506929	3.0327278
H	1.1800282	2.4542296	2.9889114
C	-0.5144177	2.9110409	4.2685281
H	0.0935154	2.9124544	5.1859597
C	-1.8920490	3.1755194	4.3359765
H	-2.3694927	3.3809038	5.3058444
C	-2.6573143	3.1803128	3.1574753
H	-3.7368384	3.3900695	3.1991365
C	-2.0509740	2.9102975	1.9217601
H	-2.6585837	2.9116601	1.0039407

S4

75

SCF Energy = -4548.301893086

C	3.9918152	0.3766472	-1.8903994
C	2.8334422	0.2313909	-1.0798070
C	1.5673339	0.2448154	-1.7145087
C	1.4841654	0.3180468	-3.1185696
C	2.6436368	0.4117292	-3.9043459
C	3.9030868	0.4597557	-3.2816225

C	2.9667063	0.1357014	0.3824488
C	4.0183049	-0.3509961	1.1170863
C	5.1957381	-1.1170429	0.6681930
C	6.4646334	-0.8999196	1.2573870
C	7.5759547	-1.6600859	0.8623150
C	7.4417750	-2.6559021	-0.1186830
C	6.1816152	-2.8938279	-0.6973359
C	5.0707938	-2.1364415	-0.3072750
Br	-0.8777635	2.4779271	-1.6501381
C	1.8479869	0.6732372	1.2762888
C	1.6418363	2.1909394	1.1127605
C	0.5736950	-0.1286716	1.0602143
C	2.3530469	0.3188384	2.7183756
C	3.8626152	0.0344594	2.5803301
O	4.6947647	1.1588139	2.9089072
H	4.1946021	-0.7671781	3.2717694
H	2.1565360	1.1338095	3.4414748
H	1.8473512	-0.5925138	3.0994310
H	0.7584734	-1.2030686	1.2376474
H	-0.2586203	0.2290521	1.6978435
H	2.5520359	2.7370370	1.4321646
H	0.7962339	2.5357224	1.7423763
H	1.4147536	2.4652990	0.0651242
H	4.6173091	1.7805969	2.1582254
H	6.5621979	-0.1139533	2.0207985
H	8.5565845	-1.4709041	1.3255441
H	8.3142862	-3.2512255	-0.4281176
H	6.0634993	-3.6826497	-1.4560595
H	4.0850026	-2.3303924	-0.7549218
H	0.0196282	-1.3477458	-0.7709208
H	0.5002402	0.3362464	-3.6123289
H	2.5576815	0.4797482	-4.9998249
H	4.8175612	0.5744735	-3.8828608
H	4.9749274	0.4326411	-1.4027165
Pd	-0.2602943	0.1627392	-0.8217188
P	-2.5265826	-0.0572432	0.0162144
C	-2.6934962	0.8098613	1.6274319
C	-3.0585753	0.1323972	2.8083251
H	-3.3226374	-0.9344189	2.7718504
C	-3.0817033	0.8206507	4.0330603
H	-3.3658920	0.2857345	4.9519332
C	-2.7445480	2.1824178	4.0850379
H	-2.7614628	2.7179397	5.0463506
C	-2.3816487	2.8594372	2.9067958
H	-2.1133658	3.9261650	2.9416814
C	-2.3484235	2.1799515	1.6812562

H	-2.0389499	2.6970110	0.7575350
C	-3.1160368	-1.7616967	0.3798861
C	-4.4886727	-2.0865537	0.3515854
H	-5.2258951	-1.3207957	0.0678968
C	-4.9114947	-3.3839411	0.6791531
H	-5.9835500	-3.6310287	0.6505559
C	-3.9714500	-4.3644725	1.0394056
H	-4.3059046	-5.3814837	1.2942105
C	-2.6032193	-4.0468833	1.0648414
H	-1.8619233	-4.8130692	1.3373938
C	-2.1763623	-2.7526313	0.7303565
H	-1.1041039	-2.5067777	0.7328687
C	-3.8454563	0.6358208	-1.0448882
C	-4.9103476	1.3961627	-0.5251688
H	-4.9524793	1.6173826	0.5514685
C	-5.9097287	1.8791840	-1.3859861
H	-6.7373674	2.4787290	-0.9777394
C	-5.8510283	1.6020621	-2.7610552
H	-6.6328847	1.9855932	-3.4338506
C	-4.7874964	0.8429582	-3.2805408
H	-4.7323251	0.6345378	-4.3594528
C	-3.7836125	0.3662504	-2.4276248
H	-2.9364375	-0.2059979	-2.8360046

Optimized Geometries(BXn(TS-df))

R3
75
SCF Energy = -4548.291180302

C	-1.6782502	4.6480355	1.8948365
C	-0.8650336	4.2193285	0.8130627
C	-0.7782049	5.0280407	-0.3420525
C	-1.5282744	6.2056211	-0.4416908
C	-2.4017942	6.5711684	0.5971424
C	-2.4942262	5.7881773	1.7599722
C	-0.3128997	2.8766497	0.9405318
C	0.8615912	2.2786615	0.6021886
C	2.0407765	2.8776226	-0.0387624
C	2.8795574	2.0981336	-0.8710029
C	4.0193491	2.6617182	-1.4640747
C	4.3500448	4.0067193	-1.2298275
C	3.5352386	4.7839942	-0.3863065
C	2.3951184	4.2265328	0.2040645

Br	1.3919320	3.5731792	3.7588012
C	-1.2814048	1.9305437	1.6588236
C	-2.3579829	1.4413351	0.6606429
C	-1.9877746	2.6998561	2.7817321
C	-0.3253327	0.7881296	2.0847534
C	0.8393251	0.8227818	1.0597130
O	0.7027379	-0.0934886	-0.0416107
H	1.7994256	0.5412525	1.5383042
H	0.0926069	1.0239922	3.0835576
H	-0.8057213	-0.2096915	2.1186545
H	-1.7628448	2.2797322	3.7954961
H	-3.0806013	2.7775491	2.6690382
H	-1.9009255	0.8661342	-0.1689512
H	-2.9093412	2.2976085	0.2218810
H	-3.0868527	0.7765976	1.1684739
H	0.0354537	0.2931399	-0.6405345
H	2.6118218	1.0461155	-1.0500086
H	4.6573545	2.0426263	-2.1135630
H	5.2475295	4.4457389	-1.6917739
H	3.8048861	5.8299340	-0.1712607
H	1.7796068	4.8162863	0.8950989
H	-0.1336265	4.6986517	-1.1701211
H	-1.4542842	6.8289188	-1.3452141
H	-3.0089726	7.4852116	0.5171909
H	-3.1621218	6.1033584	2.5721157
H	-2.4598218	4.7866521	4.2801511
Pd	-1.0294234	4.3510625	3.8683603
P	-0.3445988	6.2914547	4.9239600
C	-0.0837702	7.4280484	3.5050987
C	0.7963794	7.0089538	2.4821617
H	1.3413273	6.0573743	2.5976180
C	0.9465742	7.7887319	1.3296428
H	1.6200748	7.4487407	0.5289683
C	0.2212903	8.9848656	1.1846507
H	0.3321887	9.5886291	0.2712581
C	-0.6515737	9.4020363	2.2008850
H	-1.2221896	10.3367380	2.0909268
C	-0.8086624	8.6260010	3.3619054
H	-1.5003505	8.9512476	4.1524615
C	1.2240706	6.3014613	5.8625498
C	1.4114701	5.3119521	6.8489088
H	0.6477127	4.5327853	6.9923102
C	2.5787453	5.3097818	7.6229228
H	2.7251387	4.5327275	8.3879268
C	3.5703184	6.2831285	7.4060384
H	4.4924350	6.2718668	8.0066361

C	3.3898175	7.2614117	6.4156667
H	4.1679291	8.0191458	6.2381924
C	2.2168354	7.2749078	5.6428166
H	2.0762428	8.0365756	4.8618167
C	-1.5064892	7.2064588	6.0196988
C	-1.0186497	8.1794558	6.9188033
H	0.0644008	8.3496301	7.0071166
C	-1.9130884	8.9266049	7.7001146
H	-1.5241145	9.6804477	8.4012176
C	-3.2975625	8.7128310	7.5908858
H	-3.9963529	9.2987557	8.2069491
C	-3.7869985	7.7421054	6.7012720
H	-4.8694047	7.5623711	6.6181820
C	-2.8942485	6.9885452	5.9242149
H	-3.2682472	6.2103344	5.2387588

R4

75

SCF Energy = -4548.270695756

C	4.2163593	0.9612720	-0.2210436
C	2.8037558	0.9031780	-0.1981911
C	2.1662624	-0.1908686	-0.8294999
C	2.9148839	-1.1742739	-1.4915711
C	4.3171392	-1.0887873	-1.5298797
C	4.9640972	-0.0192819	-0.8883504
C	2.0270257	1.9081491	0.5546616
Pd	-1.9535198	4.9838007	-0.1272497
P	-2.7755323	7.0640996	0.4195671
C	0.9367646	2.6492516	0.1929109
Br	-0.2890865	6.1064739	-1.7276074
C	0.0738662	2.6387925	-0.9851535
C	0.3926832	2.0409929	-2.2256294
C	-0.5986712	1.8151612	-3.1888485
C	-1.9404427	2.1219506	-2.9060736
C	-2.2775554	2.7492530	-1.6912772
C	-1.2527023	3.1146265	-0.7970408
C	2.3374710	2.1332235	2.0412773
O	2.8433399	0.9972733	2.7159255
C	0.9805497	2.6585283	2.5749773
C	0.4086340	3.4638024	1.3738465
C	-1.1104069	3.4679286	1.3211276
C	0.9951691	4.8931266	1.4109168
H	3.1246438	2.9113259	2.1705156
H	1.0700342	3.2550454	3.5045271
H	0.3439915	1.7720393	2.7860059
H	-1.5628961	2.4692941	1.4491400

H	-1.5511395	4.1597372	2.0655776
H	0.5479935	5.4722111	2.2448145
H	0.8035110	5.4347457	0.4662673
H	2.0915757	4.8600472	1.5650518
H	2.3183916	0.2301952	2.4144951
H	1.0692690	-0.2648380	-0.7913808
H	2.3993985	-2.0175613	-1.9763231
H	4.9050789	-1.8598348	-2.0504729
H	6.0625350	0.0495344	-0.9039349
H	4.7285592	1.7910652	0.2877159
H	-3.2274072	4.4385495	0.5746534
H	-3.3277546	3.0059563	-1.4856712
H	-2.7323419	1.8895105	-3.6344441
H	-0.3285563	1.3560620	-4.1515732
H	1.4290786	1.7341470	-2.4193945
C	-2.9199925	8.2918986	-0.9269448
C	-1.5699271	7.7609581	1.6183069
C	-4.3832413	7.1938102	1.3177683
C	-5.0872192	8.4159779	1.3615528
C	-6.2714860	8.5216857	2.1062472
C	-6.7618768	7.4142369	2.8186026
C	-6.0667899	6.1947938	2.7766887
C	-4.8867318	6.0846709	2.0245944
H	-4.7129588	9.2863670	0.8038130
H	-6.8166030	9.4774922	2.1273171
H	-7.6918379	7.5001258	3.4008192
H	-6.4484617	5.3201204	3.3246513
H	-4.3473211	5.1252237	1.9707605
C	-2.6487153	9.6595342	-0.7227380
C	-2.8204124	10.5709708	-1.7772628
C	-3.2640571	10.1215871	-3.0315414
C	-3.5294922	8.7564405	-3.2364247
C	-3.3507677	7.8408538	-2.1907453
H	-2.2880699	10.0095449	0.2559810
H	-2.6006560	11.6374407	-1.6175935
H	-3.3927671	10.8370527	-3.8578481
H	-3.8593229	8.3994397	-4.2234196
H	-3.5196408	6.7659691	-2.3544431
C	-1.8362253	7.7354633	3.0025924
C	-0.8512464	8.1498262	3.9137589
C	0.3967870	8.5961629	3.4497071
C	0.6604357	8.6242467	2.0689759
C	-0.3119370	8.2019393	1.1522964
H	-2.8148598	7.3933689	3.3700274
H	-1.0645266	8.1264026	4.9932131
H	1.1673233	8.9201229	4.1656665

H	1.6397443	8.9640561	1.6996499
H	-0.0897618	8.1674877	0.0741698

S3

75

SCF Energy = -4548.267382916

C	-1.7776425	4.3857301	0.7303083
C	-1.4182078	3.0915475	0.2437730
C	-1.7564745	2.6860694	-1.0535469
C	-2.4918574	3.5555401	-1.8792792
C	-2.9050437	4.8079082	-1.3896227
C	-2.5728471	5.2190377	-0.0878237
C	-0.7285216	2.3893070	1.3314190
C	0.5923727	2.1100943	1.5205021
C	1.6830263	1.9806857	0.5352451
C	1.6706002	2.6693265	-0.7009318
C	2.7382607	2.5389892	-1.5977204
C	3.8379533	1.7217890	-1.2846100
C	3.8685453	1.0398041	-0.0570950
C	2.8042531	1.1741812	0.8457989
Br	1.6160365	5.9583038	0.5843747
C	-1.5126285	2.5528021	2.6461543
C	-2.6588776	1.5278001	2.7272947
C	-2.1074220	3.9806835	2.6253780
C	-0.4168196	2.2961610	3.7220003
C	0.9029089	2.4430074	2.9698008
O	1.2191584	3.8764476	2.9639991
H	1.7608007	1.9128134	3.4317861
H	-0.4693963	2.9909428	4.5824996
H	-0.5025037	1.2642584	4.1160976
H	-1.9723568	4.4909683	3.6030980
H	-3.1902196	4.0116579	2.4177344
H	-2.2670980	0.4912865	2.6846077
H	-3.3632640	1.6634011	1.8812736
H	-3.2242149	1.6508704	3.6746159
H	1.7671449	4.1170844	2.1624750
H	0.8391847	3.3448789	-0.9361759
H	2.7188533	3.1008126	-2.5436200
H	4.6755212	1.6248969	-1.9921590
H	4.7269389	0.4005060	0.1999821
H	2.8315935	0.6312182	1.8032670
H	-1.4520934	1.6907652	-1.4098708
H	-2.7652014	3.2447710	-2.8985885
H	-3.5012746	5.4767116	-2.0293403
H	-2.9195576	6.1966765	0.2793584
H	-1.2641929	6.5540244	1.7084562

Pd	-0.4249465	5.3719631	2.1028396
P	0.1601192	6.7383612	3.9789208
C	-0.7209512	8.3466822	4.0093506
C	-0.7936008	9.0690255	2.7984677
H	-0.3555463	8.6385078	1.8832748
C	-1.4085962	10.3291618	2.7672333
H	-1.4585364	10.8876588	1.8203974
C	-1.9639532	10.8725657	3.9388856
H	-2.4547429	11.8572345	3.9109154
C	-1.8903704	10.1577043	5.1460312
H	-2.3196677	10.5822527	6.0663244
C	-1.2630298	8.9018099	5.1861643
H	-1.1934744	8.3495795	6.1350871
C	1.9029964	7.2112681	4.3122171
C	2.9180196	6.2405243	4.1658526
H	2.6488244	5.2188051	3.8668064
C	4.2570503	6.5834574	4.4023057
H	5.0408600	5.8200382	4.2844300
C	4.5991401	7.8962399	4.7662546
H	5.6522645	8.1653217	4.9389865
C	3.5933902	8.8673506	4.8985925
H	3.8542968	9.8996795	5.1771929
C	2.2499944	8.5297469	4.6731838
H	1.4700445	9.2977797	4.7739684
C	-0.4069532	5.8370591	5.4675351
C	0.4927412	5.1456022	6.3058298
H	1.5756445	5.2801333	6.1724021
C	0.0097578	4.2867663	7.3051692
H	0.7226404	3.7543033	7.9529952
C	-1.3726898	4.1068901	7.4833647
H	-1.7466852	3.4304303	8.2663796
C	-2.2752935	4.7986605	6.6577598
H	-3.3598782	4.6705756	6.7939479
C	-1.7989705	5.6508701	5.6503741
H	-2.5119951	6.1912878	5.0082568

S4

75

SCF Energy = -4548.271411494

C	0.3609562	3.5261089	-1.8800841
C	0.1833923	3.3964797	-0.4846033
C	-1.1425016	3.4198774	0.0259345
C	-2.2428258	3.2832114	-0.8427016
C	-2.0386684	3.3770775	-2.2331999
C	-0.7416894	3.5508769	-2.7435739
C	1.2354453	3.0561493	0.4712860

C	2.4279133	2.3982339	0.3279780
C	3.1322863	1.9296152	-0.8824612
C	4.5281730	2.1255993	-1.0097439
C	5.2199901	1.6398329	-2.1294782
C	4.5368199	0.9354569	-3.1341630
C	3.1555184	0.7072837	-3.0033743
C	2.4604944	1.1957447	-1.8889879
Br	-0.9909832	6.6613006	0.5293082
C	0.8303806	3.1956797	1.9373312
C	1.1311619	4.5969317	2.5148263
C	-0.6482473	2.8486500	2.0374946
C	1.7550142	2.1440579	2.6175854
C	3.0099977	2.0923192	1.7075143
O	4.0624830	2.9983934	2.0706414
H	3.4874521	1.0910423	1.7342902
H	2.0094630	2.3927746	3.6665100
H	1.2740843	1.1439033	2.6030731
H	-0.8824112	1.8118480	1.7409792
H	-1.0518859	3.0345662	3.0521746
H	2.2229928	4.7425556	2.6295505
H	0.6811483	4.7014545	3.5234682
H	0.7318107	5.4030259	1.8713463
H	3.7675817	3.8879356	1.7941592
H	5.0603312	2.6606860	-0.2096245
H	6.3040757	1.8108001	-2.2153136
H	5.0801854	0.5546274	-4.0122845
H	2.6154435	0.1356720	-3.7737965
H	1.3837187	0.9997185	-1.7832297
H	-3.0218445	3.4411553	2.0390301
H	-3.2650878	3.1662397	-0.4521981
H	-2.9042490	3.3286867	-2.9114064
H	-0.5842412	3.6613182	-3.8268097
H	1.3804044	3.5824435	-2.2848940
Pd	-2.0570783	4.5584862	1.5551373
P	-3.2665891	5.8998900	2.9841157
C	-2.1710363	6.3521376	4.3896618
C	-2.4511713	5.9414164	5.7086306
H	-3.3692753	5.3779677	5.9289036
C	-1.5559559	6.2561215	6.7445843
H	-1.7787110	5.9317612	7.7724250
C	-0.3865087	6.9833104	6.4714389
H	0.3127216	7.2283014	7.2853480
C	-0.1097641	7.3954945	5.1555797
H	0.8071933	7.9624870	4.9346400
C	-0.9907066	7.0780237	4.1129780
H	-0.7672584	7.3713856	3.0731949

C	-4.7575046	5.2010123	3.8143462
C	-5.7974651	6.0446203	4.2583340
H	-5.7513546	7.1245497	4.0566200
C	-6.8940145	5.5071743	4.9504168
H	-7.7043708	6.1723991	5.2849240
C	-6.9595672	4.1287195	5.2123290
H	-7.8213624	3.7099477	5.7537104
C	-5.9261860	3.2845427	4.7723876
H	-5.9741397	2.2025333	4.9672281
C	-4.8343488	3.8179533	4.0710795
H	-4.0315480	3.1579846	3.7053468
C	-3.8634938	7.4871553	2.2990332
C	-3.8298310	8.6789494	3.0480403
H	-3.3916393	8.6822035	4.0570557
C	-4.3443571	9.8640461	2.4968436
H	-4.3101769	10.7964617	3.0804427
C	-4.8938494	9.8597628	1.2048003
H	-5.2912480	10.7908667	0.7731388
C	-4.9241977	8.6695834	0.4567415
H	-5.3383805	8.6677623	-0.5625211
C	-4.4038706	7.4865507	0.9973694
H	-4.3904109	6.5603005	0.4033112

Optimized Geometries(BXnf)

R3
75
SCF Energy = -4548.353461584

C	-2.3363214	4.2485956	0.9700810
C	-1.1627403	3.6435489	0.4202291
C	-0.7160170	3.9896183	-0.8659519
C	-1.4096925	4.9695552	-1.5952336
C	-2.5319039	5.6113057	-1.0461080
C	-3.0099621	5.2611501	0.2427119
C	-0.6618460	2.7048548	1.4233862
C	0.5438787	2.3023645	1.9190518
C	1.8986365	2.6359615	1.4598216
C	2.9796693	1.7611633	1.7263951
C	4.2886540	2.1187307	1.3693812
C	4.5415912	3.3532778	0.7466094
C	3.4739737	4.2314431	0.4873631
C	2.1673195	3.8786393	0.8393065
Br	0.5688911	7.0695680	0.1483110

C	-1.8428511	2.2910484	2.3084891
C	-2.6324227	1.1262507	1.6740565
C	-2.7124440	3.5857736	2.2943587
C	-1.1330164	1.8655094	3.6128222
C	0.3023659	1.4579756	3.1721179
O	0.4745307	0.0537922	2.9238652
H	1.0421223	1.6897457	3.9672730
H	-1.0626174	2.7335909	4.3013207
H	-1.6317639	1.0407527	4.1589767
H	-2.4379751	4.2419417	3.1447653
H	-3.8023648	3.3909378	2.3679662
H	-2.0067130	0.2144010	1.5989826
H	-2.9833821	1.3879166	0.6550100
H	-3.5182756	0.8756913	2.2931544
H	0.1336193	-0.1097491	2.0235950
H	2.7732069	0.7938609	2.2089763
H	5.1186864	1.4262617	1.5789643
H	5.5705159	3.6337199	0.4731762
H	3.6516343	5.2169922	0.0313881
H	1.3648816	4.6153396	0.6856822
H	0.1781776	3.5102793	-1.2878120
H	-1.0540053	5.2580841	-2.5941130
H	-3.0522178	6.3926524	-1.6185618
H	-3.9565390	5.6815754	0.6148454
H	-2.6433078	6.5823452	2.6074870
Pd	-1.4009000	6.5934751	1.6709308
P	-0.3711104	7.1937703	3.5321007
C	-0.1002543	9.0033797	3.7151578
C	0.2544973	9.7474557	2.5685908
H	0.3454540	9.2335065	1.5960498
C	0.4946895	11.1249428	2.6786838
H	0.7775592	11.6972162	1.7822269
C	0.3638752	11.7721753	3.9191707
H	0.5440228	12.8550551	3.9992682
C	-0.0076837	11.0355253	5.0554751
H	-0.1221021	11.5380183	6.0279543
C	-0.2387334	9.6541333	4.9586926
H	-0.5335869	9.0870339	5.8527838
C	1.2890366	6.4142052	3.6066682
C	1.3752551	5.0534090	3.9681966
H	0.4615905	4.4875697	4.2023856
C	2.6247290	4.4227586	4.0325621
H	2.6892146	3.3625405	4.3142008
C	3.7903236	5.1341117	3.7074113
H	4.7661258	4.6284906	3.7370512
C	3.7019990	6.4811890	3.3211373

H	4.6113473	7.0393506	3.0525137
C	2.4567266	7.1256349	3.2715919
H	2.3924064	8.1807694	2.9724930
C	-1.1121214	6.6724443	5.1387912
C	-0.2814843	6.5501441	6.2764495
H	0.8002652	6.7267948	6.1870281
C	-0.8307644	6.1931042	7.5166925
H	-0.1737435	6.0949218	8.3940095
C	-2.2108293	5.9566318	7.6375249
H	-2.6382041	5.6692611	8.6100842
C	-3.0408490	6.0811551	6.5119903
H	-4.1217905	5.8939062	6.5972486
C	-2.4924796	6.4353723	5.2692958
H	-3.1341311	6.5220485	4.3773898

R4

75

SCF Energy = -4548.346461001

C	4.4288726	1.4136278	-0.0700892
C	3.0329714	1.2300438	-0.2327702
C	2.5887586	0.4021147	-1.2929760
C	3.4996714	-0.1869363	-2.1790278
C	4.8801905	0.0302587	-2.0234756
C	5.3382875	0.8278428	-0.9615771
C	2.0859766	1.8495326	0.7036840
Pd	-2.4660388	4.8848251	-0.4111033
P	-2.8208041	6.9749987	0.2454564
C	0.8080061	2.2837215	0.4986851
Br	-0.5890874	5.5778106	-1.9624172
C	-0.2139274	2.2994633	-0.5454364
C	-0.1389074	2.2464515	-1.9490010
C	-1.3206467	2.2950814	-2.7093081
C	-2.5724141	2.3922638	-2.0864920
C	-2.6734257	2.4509749	-0.6680485
C	-1.4842972	2.4170887	0.0998028
C	2.4408810	2.0472077	2.1900826
O	3.2889543	1.0520836	2.7365560
C	1.0469777	2.1541816	2.8677965
C	0.1697217	2.8167029	1.7888286
C	-1.3179246	2.4033741	1.6124867
C	0.2775217	4.3559343	1.8418536
H	3.0038978	2.9992131	2.3275645
H	1.0777026	2.6993490	3.8320244
H	0.6942649	1.1184231	3.0655842
H	-1.4803285	1.3681199	1.9891114
H	-2.0345101	3.0695787	2.1311823

H	-0.2195577	4.7573236	2.7482568
H	-0.2060165	4.8118891	0.9539985
H	1.3333670	4.6900650	1.8467088
H	2.9384852	0.1890717	2.4417687
H	1.5132422	0.2025607	-1.4016406
H	3.1301578	-0.8287190	-2.9936223
H	5.5963208	-0.4306017	-2.7205784
H	6.4177659	0.9933089	-0.8233218
H	4.7995891	2.0196776	0.7676120
H	-3.6396251	4.5566605	0.5593110
H	-3.6560933	2.3691107	-0.1821422
H	-3.4899249	2.4224004	-2.6921187
H	-1.2589273	2.2869950	-3.8068544
H	0.8371162	2.1973816	-2.4498238
C	-2.7717996	8.2078564	-1.1082865
C	-1.5283513	7.5094602	1.4378122
C	-4.3953216	7.3679635	1.1250961
C	-4.9529872	8.6610942	1.0382752
C	-6.1049749	8.9827144	1.7730477
C	-6.7045402	8.0240499	2.6059708
C	-6.1517167	6.7355378	2.6964425
C	-5.0076959	6.4077884	1.9536226
H	-4.4885909	9.4179665	0.3901370
H	-6.5374268	9.9912910	1.6902013
H	-7.6087530	8.2785447	3.1794056
H	-6.6195897	5.9762138	3.3410967
H	-4.5814836	5.3928778	2.0006238
C	-2.2045955	9.4843288	-0.9287895
C	-2.2351641	10.4151912	-1.9802650
C	-2.8341785	10.0771092	-3.2042104
C	-3.4002970	8.8022913	-3.3817982
C	-3.3646819	7.8662276	-2.3401711
H	-1.7296501	9.7463536	0.0280236
H	-1.7828384	11.4088213	-1.8414136
H	-2.8517543	10.8066302	-4.0280656
H	-3.8567781	8.5296517	-4.3450393
H	-3.7728467	6.8538256	-2.4807100
C	-1.8382571	7.7870761	2.7841812
C	-0.8138926	8.1327158	3.6811916
C	0.5160527	8.2110376	3.2384183
C	0.8229573	7.9388720	1.8933461
C	-0.1895182	7.5806475	0.9937708
H	-2.8791408	7.7347546	3.1343628
H	-1.0609598	8.3448479	4.7324732
H	1.3166037	8.4817180	3.9435769
H	1.8644648	7.9914586	1.5418109

H	0.0493422	7.3194890	-0.0509891
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S3

75

SCF Energy = -4548.352558334

C	-1.9694485	2.9866875	1.6629532
C	-1.1700308	2.9792096	0.4778385
C	-1.5705368	3.7358131	-0.6433042
C	-2.7235968	4.5328429	-0.5692432
C	-3.5020850	4.5680351	0.5983823
C	-3.1444388	3.7746842	1.7246645
C	0.1145620	2.3878990	0.8247085
C	1.4058736	2.6883958	0.4738455
C	1.8700511	3.1245535	-0.8450209
C	1.2287805	2.6150935	-2.0041582
C	1.6297848	3.0061040	-3.2881270
C	2.6982896	3.9049911	-3.4486626
C	3.3648635	4.3944838	-2.3120059
C	2.9616336	4.0120111	-1.0260919
Br	0.3108388	5.9078497	1.2791702
C	0.0307921	1.7140491	2.1946869
C	0.1036687	0.1815767	2.0394130
C	-1.3482531	2.1541934	2.7705372
C	1.3007478	2.2711122	2.8797594
C	2.2928986	2.6199386	1.7294593
O	2.9510465	3.8636010	1.9579432
H	3.1100290	1.8712485	1.6312168
H	1.0505185	3.2233827	3.3871396
H	1.7362064	1.5919836	3.6397057
H	-1.2489699	2.7439715	3.7049957
H	-1.9894035	1.2801035	3.0153794
H	1.0564934	-0.1221903	1.5604658
H	-0.7260919	-0.1954358	1.4065939
H	0.0375034	-0.3164334	3.0297512
H	2.2361860	4.5501290	1.9161016
H	0.4253936	1.8733410	-1.8791593
H	1.1154877	2.5947635	-4.1704723
H	3.0172798	4.2132144	-4.4560716
H	4.2080982	5.0927490	-2.4285983
H	3.4721249	4.3987275	-0.1347503
H	-0.9536335	3.7448744	-1.5512473
H	-3.0100135	5.1522983	-1.4317854
H	-4.4137195	5.1821133	0.6397815
H	-3.8419270	3.6693747	2.5677250
H	-2.8383027	5.2679867	3.8214148
Pd	-1.6824359	5.4347351	2.7950776

P	-0.7261557	6.5660676	4.4404285
C	-0.0652662	8.2234134	4.0126506
C	-0.5480040	8.8802985	2.8649404
H	-1.2480100	8.3550231	2.1987791
C	-0.1102376	10.1795394	2.5675162
H	-0.4854796	10.6867751	1.6662259
C	0.8157634	10.8213414	3.4060203
H	1.1655629	11.8367706	3.1654589
C	1.3008590	10.1651690	4.5503347
H	2.0299820	10.6633455	5.2070194
C	0.8576587	8.8707131	4.8594352
H	1.2412599	8.3617381	5.7559115
C	0.6838164	5.5697476	5.0472100
C	0.4354435	4.5024423	5.9379611
H	-0.5810080	4.3353093	6.3258132
C	1.4852173	3.6586415	6.3269560
H	1.2890244	2.8303583	7.0243855
C	2.7793397	3.8622414	5.8171677
H	3.5989285	3.1902836	6.1126362
C	3.0211681	4.9066754	4.9112193
H	4.0217193	5.0436891	4.4787002
C	1.9782627	5.7629488	4.5260058
H	2.1582658	6.5635917	3.7945151
C	-1.7160732	6.9357962	5.9510550
C	-1.0859213	7.1146924	7.2008198
H	-0.0048346	6.9403461	7.3042873
C	-1.8403685	7.4938515	8.3214076
H	-1.3432322	7.6191010	9.2952166
C	-3.2236909	7.7089957	8.2021449
H	-3.8132038	8.0059357	9.0827251
C	-3.8529883	7.5374702	6.9581776
H	-4.9368014	7.7003940	6.8594073
C	-3.1029718	7.1483282	5.8377904
H	-3.5911006	6.9948734	4.8627501

S4

75

SCF Energy = -4548.348016586

C	-0.1896339	3.3416333	-1.5541851
C	-0.0498103	2.7802718	-0.2724482
C	-1.1971764	2.3027390	0.4317383
C	-2.4789088	2.3688929	-0.1663003
C	-2.5964820	2.9405268	-1.4646870
C	-1.4652377	3.4185615	-2.1406043
C	1.1099265	2.5734547	0.5937045
C	2.4545293	2.3582218	0.4849439

C	3.3247295	2.3933634	-0.7001681
C	4.6791471	2.7900276	-0.5720003
C	5.5273665	2.8108579	-1.6882888
C	5.0489894	2.4252208	-2.9516026
C	3.7133624	2.0067386	-3.0875076
C	2.8612959	1.9892917	-1.9756028
Br	-1.2757558	6.1537750	-0.0554065
C	0.5955927	2.3643499	2.0255630
C	0.3750676	3.7178148	2.7345854
C	-0.7861025	1.6955037	1.7647073
C	1.7506277	1.5670631	2.6645272
C	3.0123749	2.0151934	1.8711391
O	3.7299124	3.1126450	2.4585379
H	3.7614583	1.1981177	1.8127087
H	1.8787666	1.7388297	3.7513767
H	1.5990512	0.4798164	2.5002584
H	-0.6649826	0.5955780	1.6440995
H	-1.5292969	1.8701022	2.5672170
H	1.3317247	4.2514866	2.8966577
H	-0.0944827	3.5704667	3.7283578
H	-0.2811252	4.3815739	2.1361090
H	3.2128284	3.9176946	2.2610533
H	5.0449381	3.0992760	0.4183567
H	6.5735690	3.1326180	-1.5701882
H	5.7158993	2.4426418	-3.8269594
H	3.3348064	1.6814187	-4.0688152
H	1.8282300	1.6290975	-2.0834101
H	-3.6557465	3.4637954	1.8970300
H	-3.3357509	1.8504574	0.2868919
H	-3.5877386	2.9996922	-1.9373194
H	-1.5800288	3.8860291	-3.1288765
H	0.6861718	3.7427158	-2.0817673
Pd	-2.7254940	4.4410049	1.1193248
P	-3.3637951	5.8946224	2.6719200
C	-2.0194946	6.1762587	3.8939906
C	-2.1452822	5.7664141	5.2362901
H	-3.0812187	5.3110978	5.5902536
C	-1.0711067	5.9403990	6.1247669
H	-1.1730754	5.6143646	7.1709510
C	0.1235807	6.5300571	5.6821796
H	0.9640830	6.6632546	6.3801273
C	0.2444646	6.9463528	4.3444098
H	1.1797848	7.4058916	3.9905829
C	-0.8159053	6.7648330	3.4470464
H	-0.7117322	7.0446206	2.3851987
C	-4.8135547	5.4660576	3.7306085

C	-5.6444290	6.4819315	4.2477685
H	-5.4730567	7.5303172	3.9647038
C	-6.6961738	6.1567827	5.1190336
H	-7.3449280	6.9559465	5.5083354
C	-6.9219711	4.8213176	5.4895719
H	-7.7479198	4.5693989	6.1718655
C	-6.0958339	3.8064044	4.9777426
H	-6.2707595	2.7564648	5.2570900
C	-5.0527680	4.1269525	4.0964435
H	-4.4165884	3.3342582	3.6714637
C	-3.7801001	7.5553287	2.0219818
C	-3.4737352	8.7281183	2.7394571
H	-2.9289343	8.6639431	3.6928546
C	-3.8539121	9.9790059	2.2261377
H	-3.6050548	10.8950091	2.7830492
C	-4.5421779	10.0602518	1.0049667
H	-4.8339621	11.0421379	0.6024508
C	-4.8473315	8.8886688	0.2899802
H	-5.3727622	8.9510337	-0.6746615
C	-4.4624981	7.6385747	0.7920247
H	-4.6639918	6.7182915	0.2230032

Optimized Geometries (BXni)

R3
79
SCF Energy = -2238.417427572

C	-1.3225238	2.7342787	2.4227937
C	-0.1033371	2.2554442	1.8924999
C	0.9602344	1.9462334	2.7631374
C	0.7964421	2.0854315	4.1501749
C	-0.4198057	2.5510666	4.6747096
C	-1.4748555	2.8876338	3.8079905
P	0.0264890	1.9473095	0.0926023
C	1.8062497	1.6073390	-0.1848025
C	2.2333151	0.2684425	-0.2753874
C	3.5952420	-0.0278155	-0.4278964
C	4.5331633	1.0148470	-0.4949941
C	4.1078523	2.3540119	-0.4168553
C	2.7463415	2.6554023	-0.2635701
Pd	-1.0996581	0.2577127	-0.8101327
O	-0.2540005	0.6910990	-2.7232740
C	0.7220867	-0.0050318	-3.1962781

O	1.1683636	-1.0856343	-2.7730782
C	-1.4891442	-2.3299335	-1.5616782
C	-1.7572747	-2.9319805	-0.3093774
C	-2.7310356	-3.9499471	-0.2492958
C	-3.4280333	-4.3366963	-1.4062530
C	-3.1787394	-3.7045328	-2.6372125
C	-2.1997241	-2.7018081	-2.7150598
C	-1.1249346	-2.3525353	0.8992545
C	0.1583507	-2.4556335	1.3296740
C	0.4320966	-1.4289527	2.4315207
C	-0.9628305	-0.9870752	2.8724235
C	-1.9299913	-1.3159342	1.7039640
C	1.2523028	-3.3079366	0.8154420
C	1.9083409	-4.1922505	1.7087606
C	2.9873194	-4.9789753	1.2770467
C	3.4354531	-4.8941182	-0.0517531
C	2.7918712	-4.0205882	-0.9439677
C	1.7091607	-3.2335336	-0.5206278
C	-3.2598931	-1.8827504	2.2483400
C	-2.2749686	-0.1079896	0.8049032
O	1.1797820	-1.8860590	3.5539615
C	-0.2668020	3.5915914	-0.6712572
C	-0.4737788	3.6551552	-2.0669621
C	-0.6354200	4.9040389	-2.6847706
C	-0.5946769	6.0865912	-1.9260671
C	-0.3829907	6.0217147	-0.5392356
C	-0.2166162	4.7782523	0.0914235
O	1.2829602	0.5722238	-4.3080889
H	1.9888938	-0.0511517	-4.5728585
H	0.9783555	-0.5814110	1.9486694
H	-1.0084201	0.0700328	3.1876772
H	-1.2196567	-1.6120818	3.7520673
H	-2.4849729	0.7818875	1.4280382
H	-3.1864843	-0.3300011	0.1967209
H	-3.0781781	-2.7779751	2.8784351
H	-3.9511182	-2.1655816	1.4297364
H	-3.7679718	-1.1196352	2.8737728
H	2.0650965	-2.1304460	3.2208203
H	1.5412825	-4.2717114	2.7426341
H	3.4764358	-5.6685330	1.9824507
H	4.2829305	-5.5097600	-0.3904510
H	3.1328874	-3.9390684	-1.9873382
H	1.2560219	-2.5335297	-1.2365043
H	-2.9385599	-4.4428044	0.7114115
H	-4.1807197	-5.1376530	-1.3440991
H	-3.7379988	-4.0053844	-3.5359190

H	-1.9618544	-2.2158702	-3.6728364
H	-0.6095259	-1.6541844	-1.6773920
H	-0.4851090	2.7207174	-2.6536994
H	-0.7952627	4.9506012	-3.7725839
H	-0.7267000	7.0628673	-2.4170400
H	-0.3446907	6.9444664	0.0594934
H	-0.0448297	4.7337050	1.1764062
H	1.4901779	-0.5394738	-0.2661294
H	3.9070641	-1.0795482	-0.5108678
H	5.6024688	0.7865303	-0.6217521
H	4.8421750	3.1710660	-0.4830369
H	2.4115876	3.7022403	-0.2116530
H	1.9145207	1.5845691	2.3552755
H	1.6242401	1.8191699	4.8235147
H	-0.5474813	2.6536303	5.7627064
H	-2.4268158	3.2609370	4.2142617
H	-2.1503598	2.9958357	1.7461067

R4

79

SCF Energy = -2238.427040432

C	1.7810942	3.7592127	1.8588095
C	0.8656017	2.6873038	1.9307594
C	0.4866750	2.1936405	3.2004867
C	1.0181494	2.7617081	4.3681409
C	1.9324619	3.8242483	4.2877873
C	2.3093884	4.3224552	3.0295297
P	0.2888408	1.8788861	0.3790140
C	-1.4304542	1.3576644	0.7544456
C	-2.2673744	2.1028852	1.6108261
C	-3.5666741	1.6478372	1.8891669
C	-4.0356094	0.4543645	1.3158961
C	-3.2099049	-0.2789797	0.4466829
C	-1.9119688	0.1707758	0.1630757
Pd	1.4610568	0.1103981	-0.3331615
C	1.4504508	-0.4563669	1.6441281
C	1.6384086	-1.9786481	1.8134576
C	0.8026993	-2.6535065	0.7095791
C	-0.3250349	-3.2453490	1.2245046
C	-0.4813526	-2.8867311	2.6974969
C	0.9437932	-2.4982433	3.1070993
C	-1.3532560	-4.0500711	0.5419140
C	-2.7180986	-3.9301839	0.9022058
C	-3.6964734	-4.7085383	0.2650079
C	-3.3336468	-5.6297584	-0.7312131
C	-1.9779655	-5.7790941	-1.0761323

C	-0.9989297	-5.0034642	-0.4439080
C	1.0885254	-2.3909246	-0.7230761
C	2.4195631	-2.1860449	-1.2108884
C	2.6690284	-1.9983008	-2.5857516
C	1.6153807	-1.9778725	-3.5023323
C	0.2947403	-2.1439646	-3.0398091
C	0.0345886	-2.3395093	-1.6845381
O	-1.4486885	-1.8324616	2.8633155
C	3.1388104	-2.3379335	1.8770564
O	-0.6281071	0.8767222	-2.5092119
C	0.1902589	3.2505692	-0.8287690
C	-1.0197574	3.9244753	-1.0820153
C	-1.0536114	4.9676544	-2.0185774
C	0.1123871	5.3335993	-2.7124737
C	1.3157060	4.6522161	-2.4694143
C	1.3597263	3.6118231	-1.5294656
H	-0.8746577	-3.7290673	3.3036828
H	1.4709065	-3.4055680	3.4702417
H	0.9516324	-1.7499603	3.9239523
H	0.4792819	-0.1827277	2.0989292
H	2.2372073	0.1267238	2.1710112
H	3.5186712	-2.0958243	2.8909398
H	3.7525024	-1.7494070	1.1690284
H	3.3156318	-3.4178395	1.6972246
H	-1.3718502	-1.2324446	2.0916405
H	0.0614939	-5.1310417	-0.7066968
H	-1.6813235	-6.5135431	-1.8404462
H	-4.1022731	-6.2391797	-1.2302104
H	-4.7533390	-4.5949285	0.5518072
H	-2.9938404	-3.2046932	1.6814140
H	-1.0022862	-2.4453836	-1.3452919
H	-0.5478613	-2.0804647	-3.7429982
H	1.8101345	-1.7964318	-4.5686850
H	3.7032067	-1.8455297	-2.9261132
H	3.2711593	-2.2829509	-0.5307622
H	-1.9006947	3.0313485	2.0728797
H	-4.2129783	2.2271453	2.5656654
H	-5.0492677	0.0944552	1.5479312
H	-3.5716253	-1.2118920	-0.0103315
H	-1.2641422	-0.3622336	-0.5465999
H	-1.9399068	3.6189262	-0.5644016
H	-2.0022078	5.4890509	-2.2173465
H	0.0789707	6.1440367	-3.4564203
H	2.2257246	4.9175244	-3.0275337
H	2.2870292	3.0422220	-1.3769099
H	-0.2360553	1.3703391	3.2844436

H	0.7101932	2.3686592	5.3488237
H	2.3469339	4.2679958	5.2055628
H	3.0178976	5.1612943	2.9559530
H	2.0760446	4.1634778	0.8799090
C	0.5310097	1.0084320	-2.9420977
O	1.6388847	0.7818307	-2.3284754
O	0.7283365	1.4543750	-4.2301738
H	-0.1779923	1.6168469	-4.5601094

S3

79

SCF Energy = -2238.447495460

C	-1.1684261	-1.5839154	2.0392392
C	0.0987336	-1.0763137	2.3949030
C	0.9893830	-1.8777563	3.1371762
C	0.6111917	-3.1737224	3.5234073
C	-0.6563280	-3.6719195	3.1800111
C	-1.5449118	-2.8728318	2.4400823
P	0.6010052	0.5774594	1.7843416
C	1.8807972	1.1082825	2.9950865
C	3.2144073	1.2434648	2.5606455
C	4.2172458	1.6145087	3.4710666
C	3.8909125	1.8584273	4.8146591
C	2.5592156	1.7322073	5.2492768
C	1.5554544	1.3582171	4.3445437
Pd	1.3503506	0.7999292	-0.2921795
C	2.1852236	-1.0584319	-0.2772557
C	1.4392502	-2.1031105	-1.1726611
C	0.3311445	-1.4167568	-2.0202399
C	0.7841322	-1.1181122	-3.2776855
C	2.2090311	-1.6448443	-3.4836432
C	2.3827845	-2.6125113	-2.2957764
C	-1.0279524	-1.1514700	-1.4713959
C	-1.5011423	0.1518795	-1.1856159
C	-2.7836482	0.3564516	-0.6541417
C	-3.6392503	-0.7338970	-0.4242682
C	-3.1998325	-2.0312694	-0.7368890
C	-1.9075044	-2.2363514	-1.2452127
C	0.1183406	-0.3327255	-4.3328749
C	0.9183328	0.3425115	-5.2965036
C	0.3327067	1.1456167	-6.2874069
C	-1.0636956	1.2914113	-6.3508696
C	-1.8668063	0.6013989	-5.4279805
C	-1.2879518	-0.2028530	-4.4364565
C	0.9400321	-3.2665654	-0.3057176
O	3.2087265	-0.6323731	-3.5553845

O	2.0235237	1.3935548	-2.2826144
C	-0.8675080	1.6283272	2.1380111
C	-1.0782755	2.7812718	1.3534293
C	-2.1853851	3.6063168	1.6075470
C	-3.0861999	3.2901076	2.6375774
C	-2.8760095	2.1433527	3.4219039
C	-1.7716178	1.3138309	3.1758445
H	2.2664374	-2.2004384	-4.4473984
H	3.4437012	-2.6840698	-1.9862852
H	2.0463144	-3.6265106	-2.5993733
H	3.1574388	-0.7734810	-0.7314750
H	2.3623026	-1.4617544	0.7384492
H	0.4623157	-4.0527967	-0.9248145
H	0.2108763	-2.9336751	0.4526238
H	1.7947635	-3.7319115	0.2258552
H	2.8540713	0.1687098	-3.0956173
H	2.0120238	0.2309739	-5.2385004
H	0.9749041	1.6591951	-7.0200606
H	-1.5228737	1.9272817	-7.1226114
H	-2.9629651	0.6872968	-5.4807147
H	-1.9370011	-0.7470904	-3.7392776
H	-1.5774441	-3.2540110	-1.4936017
H	-3.8659129	-2.8938179	-0.5816004
H	-4.6461527	-0.5715644	-0.0110579
H	-3.1097821	1.3798874	-0.4179802
H	-0.8690390	1.0263583	-1.3910520
H	-0.3974389	3.0197755	0.5237154
H	-2.3457199	4.4991268	0.9847118
H	-3.9569192	3.9357244	2.8285393
H	-3.5792815	1.8879762	4.2290658
H	-1.6261277	0.4077695	3.7816449
H	3.4495925	1.0628412	1.4991018
H	5.2565343	1.7194600	3.1252382
H	4.6756471	2.1546605	5.5272086
H	2.3004512	1.9308923	6.3003179
H	0.5141076	1.2678310	4.6874084
H	1.9776846	-1.4852630	3.4186678
H	1.3122442	-3.7962587	4.0994456
H	-0.9507648	-4.6869477	3.4865036
H	-2.5350706	-3.2572139	2.1539344
H	-1.8597809	-0.9734710	1.4422108
C	1.2258573	2.4061385	-2.2981201
O	0.6788975	2.8233217	-1.2392871
O	0.9387760	3.0033880	-3.4619566
H	1.2360960	2.4034922	-4.1862377

S4
79
SCF Energy = -2238.429904093

C	-1.4763787	4.0962215	-1.3861767
C	-0.9848367	3.8914474	-0.0786155
C	-1.0011303	4.9539972	0.8504206
C	-1.5020662	6.2102850	0.4730321
C	-1.9879064	6.4141972	-0.8285761
C	-1.9730871	5.3561001	-1.7531615
P	-0.2593377	2.2488002	0.3525149
C	-0.1775440	2.3375701	2.1828320
C	1.0418029	2.3815918	2.8846826
C	1.0438346	2.3924024	4.2889166
C	-0.1676917	2.3616696	4.9984933
C	-1.3879930	2.3319982	4.3001785
C	-1.3945090	2.3190379	2.8982976
Pd	-1.3623660	0.6240782	-0.6803819
C	-1.7339892	-0.5195788	0.9558756
C	-0.7356149	-1.5504449	1.5127975
C	-0.2135956	-2.6124877	0.5281100
C	-0.3548020	-3.8847185	1.0092788
C	-0.9326296	-3.8600153	2.4192509
C	-1.5111719	-2.4387752	2.5401011
C	0.5739178	-2.2474991	-0.6734558
C	1.9776566	-2.4077511	-0.6552463
C	2.7504210	-2.0806131	-1.7795368
C	2.1348414	-1.5711521	-2.9362172
C	0.7407954	-1.4110922	-2.9676277
C	-0.0360558	-1.7533364	-1.8471718
C	0.0631555	-5.1476352	0.3697946
C	0.4177501	-6.2651294	1.1669440
C	0.8022920	-7.4770189	0.5755606
C	0.8368827	-7.6061469	-0.8225431
C	0.4750848	-6.5103182	-1.6251464
C	0.0918206	-5.2973453	-1.0388580
C	0.4752007	-0.8701842	2.1830989
O	0.0721528	-4.1593654	3.4046894
O	-1.5164506	1.3265809	-2.8285803
C	1.4847401	2.3968313	-0.2009219
C	2.1359460	1.2592674	-0.7159631
C	3.4796697	1.3438112	-1.1131843
C	4.1717907	2.5605648	-1.0080565
C	3.5178558	3.7015093	-0.5093234
C	2.1761173	3.6238481	-0.1091909
H	-1.7093330	-4.6372227	2.5745309
H	-1.4370245	-2.0585331	3.5778537

H	-2.5852059	-2.4626313	2.2644170
H	-2.6177880	-1.0445365	0.5289448
H	-2.0732886	0.1199208	1.7955720
H	1.1467572	-1.6215107	2.6463823
H	0.1436983	-0.1786672	2.9793738
H	1.0738139	-0.2963042	1.4494816
H	0.8758943	-3.6741775	3.1342744
H	0.4116576	-6.1555994	2.2609525
H	1.0801276	-8.3289053	1.2153138
H	1.1384293	-8.5579961	-1.2858444
H	0.4844131	-6.6028115	-2.7220758
H	-0.2069520	-4.4568693	-1.6788686
H	-1.1321701	-1.6957594	-1.9040981
H	0.2481735	-1.0178034	-3.8687493
H	2.7413671	-1.3036253	-3.8144499
H	3.8412900	-2.2264169	-1.7516817
H	2.4562799	-2.8089111	0.2503281
H	1.5830202	0.3140066	-0.8180242
H	3.9767628	0.4502183	-1.5161566
H	5.2235550	2.6254047	-1.3260088
H	4.0542119	4.6599143	-0.4385414
H	1.6597643	4.5192374	0.2680914
H	1.9918337	2.3917657	2.3315253
H	2.0008086	2.4203877	4.8314787
H	-0.1628544	2.3632098	6.0988546
H	-2.3402853	2.3144979	4.8511483
H	-2.3491216	2.3021981	2.3499382
H	-0.6242202	4.8009068	1.8719330
H	-1.5128075	7.0332898	1.2038535
H	-2.3827172	7.3990232	-1.1214394
H	-2.3573169	5.5077818	-2.7732318
H	-1.4813898	3.2657731	-2.1094302
C	-2.4173534	0.4546445	-3.0139673
O	-2.9677695	0.3679612	-4.2459539
O	-2.8127064	-0.3495591	-2.1001202
H	-3.6282422	-0.3534007	-4.1934056

Optimized Geometries (TS-BXni-e')

R3
 79
 SCF Energy = -2238.384370682
 C -2.3079442 6.2475034 5.6941869

C	-0.9459473	6.1309523	5.3361505
C	-0.1044509	5.2750147	6.0739059
C	-0.6224891	4.5315313	7.1461170
C	-1.9777956	4.6452891	7.4954891
C	-2.8172247	5.5126273	6.7745664
P	-0.3597225	6.9705105	3.8197076
C	1.4681629	6.7687544	3.8616508
C	2.0410514	5.7424942	3.0842739
C	3.4313325	5.5590731	3.0620126
C	4.2555124	6.4065967	3.8201589
C	3.6879885	7.4346522	4.5967993
C	2.2971467	7.6205699	4.6187612
Pd	-1.0306370	6.2170727	1.7943657
O	0.3026812	7.3386059	0.2810205
C	1.6189414	7.3533404	0.4244343
O	2.4215781	6.5521170	-0.0320247
C	-1.1604147	5.1740447	-0.2449753
C	-1.0700364	3.7690624	0.0016707
C	-1.3721460	2.8499707	-1.0198561
C	-1.8010605	3.3026513	-2.2803072
C	-1.9539066	4.6766436	-2.5210009
C	-1.6313440	5.5983958	-1.5094155
C	-0.8459692	3.3103150	1.3974958
C	0.2703418	2.8129052	1.9924193
C	0.0670422	2.7331321	3.5087135
C	-1.4494943	2.8636898	3.6905437
C	-2.0266159	3.4618077	2.3767758
C	1.5857941	2.5760609	1.3676063
C	2.3569928	1.4376514	1.7135951
C	3.6357898	1.2455072	1.1685647
C	4.1728246	2.1843629	0.2710188
C	3.4118307	3.3094697	-0.0901741
C	2.1298741	3.4977091	0.4435631
C	-3.2486402	2.6531860	1.8872622
C	-2.4474217	4.9438613	2.5021551
O	0.5313016	1.5516034	4.1634240
C	-0.6224093	8.7580914	4.1285182
C	-0.5623845	9.6209277	3.0126881
C	-0.7070769	11.0037481	3.1948007
C	-0.9196710	11.5306346	4.4808465
C	-0.9824132	10.6717841	5.5907140
C	-0.8313764	9.2861370	5.4188970
O	1.9989060	8.4315950	1.1718569
H	2.9668906	8.3382015	1.2862601
H	0.5897674	3.6163396	3.9520289
H	-1.7195701	3.4524035	4.5869999

H	-1.8352246	1.8346918	3.8386129
H	-2.7494446	5.1874525	3.5370225
H	-3.2797501	5.1929967	1.8103621
H	-2.9883736	1.5811214	1.7685175
H	-3.6137697	3.0300772	0.9108295
H	-4.0785063	2.7293589	2.6202985
H	1.5021359	1.6247820	4.2193933
H	1.9228624	0.6860110	2.3881036
H	4.2152877	0.3502569	1.4427770
H	5.1799156	2.0362491	-0.1482638
H	3.8128258	4.0672135	-0.7792317
H	1.5747745	4.4023626	0.1670773
H	-1.2892397	1.7719734	-0.8138778
H	-2.0328714	2.5737947	-3.0722777
H	-2.3092580	5.0319247	-3.5005767
H	-1.6997458	6.6782312	-1.7192152
H	-0.2213797	6.2156769	-0.0162548
H	-0.3897369	9.2034287	2.0088236
H	-0.6566708	11.6742569	2.3238025
H	-1.0390304	12.6160992	4.6184422
H	-1.1488303	11.0817297	6.5985138
H	-0.8784366	8.6131477	6.2880464
H	1.3920676	5.1136187	2.4577073
H	3.8566024	4.7677040	2.4275378
H	5.3480718	6.2741480	3.7999518
H	4.3360542	8.1032874	5.1838259
H	1.8556948	8.4368355	5.2098519
H	0.9575077	5.1870500	5.8030339
H	0.0382501	3.8548997	7.7080804
H	-2.3825173	4.0570246	8.3326065
H	-3.8786386	5.6090009	7.0482317
H	-2.9681455	6.9215124	5.1262417

R4

79

SCF Energy = -2238.398228183

C	-0.1128410	8.5967984	1.3540464
C	-1.0677323	7.5942731	1.6343705
C	-1.1794993	7.0870000	2.9433058
C	-0.3497881	7.5825991	3.9628691
C	0.5883722	8.5881474	3.6835930
C	0.7034062	9.0969986	2.3777357
P	-2.0078736	6.8778099	0.2341621
C	-3.2887289	5.8235376	1.0316233
C	-4.5563123	6.3262878	1.3845774
C	-5.5052015	5.4766765	1.9746126

C	-5.1956675	4.1273902	2.2178236
C	-3.9309921	3.6232170	1.8697205
C	-2.9816598	4.4675043	1.2763894
Pd	-0.8954483	5.4468625	-1.1683523
C	0.7917862	5.6804486	-0.0314320
C	1.9500465	4.6583473	-0.1234210
C	1.3690254	3.2691809	-0.4109831
C	1.2231013	2.5144117	0.7164912
C	1.7260945	3.3046709	1.9247385
C	2.5644017	4.4332422	1.2846034
C	0.5426162	1.2170893	0.8706442
C	0.7224152	0.4565031	2.0528846
C	0.0943770	-0.7850912	2.2206426
C	-0.7432832	-1.2967084	1.2161123
C	-0.9520633	-0.5446922	0.0467150
C	-0.3220871	0.6943182	-0.1242650
C	0.9936863	3.0265308	-1.8168805
C	1.7841255	2.2257126	-2.6630427
C	1.5232494	2.1932136	-4.0432351
C	0.4783411	2.9605718	-4.5878383
C	-0.3325741	3.7289480	-3.7396861
C	-0.0998180	3.7723441	-2.3410757
O	0.6367872	3.7544431	2.7434258
C	2.9827848	5.1029284	-1.1676993
O	-2.5199547	2.9737158	-1.5420564
C	-2.9448588	8.2923463	-0.4645111
C	-3.1332359	9.4922197	0.2538731
C	-3.8871531	10.5340480	-0.3090261
C	-4.4583933	10.3821729	-1.5838124
C	-4.2776012	9.1837806	-2.2955166
C	-3.5227820	8.1382163	-1.7442545
H	2.3491157	2.6926398	2.6095197
H	3.6121100	4.0836021	1.1691873
H	2.5733687	5.3432765	1.9170325
H	0.4232681	5.6925846	1.0131593
H	1.1520693	6.7089099	-0.2547251
H	3.4657930	6.0482567	-0.8459392
H	2.5001937	5.2812095	-2.1495996
H	3.7748481	4.3385622	-1.3057534
H	-0.0549140	4.0785651	2.1344696
H	-0.5219091	1.2737004	-1.0337693
H	-1.6214035	-0.9228343	-0.7412792
H	-1.2397603	-2.2702636	1.3482124
H	0.2590941	-1.3571314	3.1467659
H	1.3616874	0.8477622	2.8561948
H	-1.2781744	3.4742800	-1.7257055

H	-1.1929073	4.2824302	-4.1488412
H	0.2850261	2.9393258	-5.6712226
H	2.1485676	1.5686204	-4.7007913
H	2.6142357	1.6427835	-2.2368636
H	-4.8033993	7.3794831	1.1841613
H	-6.4982898	5.8706516	2.2385166
H	-5.9473527	3.4641350	2.6725758
H	-3.6807310	2.5662067	2.0445906
H	-2.0077806	4.0644891	0.9547293
H	-2.6903518	9.6115907	1.2537344
H	-4.0299611	11.4690942	0.2539181
H	-5.0477874	11.2008681	-2.0232276
H	-4.7272993	9.0595765	-3.2926559
H	-3.3961820	7.1873960	-2.2841696
H	-1.9121035	6.2979198	3.1664659
H	-0.4386411	7.1750410	4.9808134
H	1.2363233	8.9755415	4.4845153
H	1.4408074	9.8824368	2.1532266
H	-0.0117430	8.9858145	0.3287821
C	-3.2757979	3.9295311	-1.9433495
O	-2.9047958	5.1054174	-2.2084956
O	-4.5901743	3.6502140	-2.0999836
H	-4.6929793	2.7066788	-1.8597325

S3

79

SCF Energy = -2238.387563153

C	-2.5666753	5.3336687	6.0124823
C	-1.3721945	6.0788551	6.0910190
C	-0.8599683	6.4601895	7.3490027
C	-1.5489796	6.1050977	8.5185622
C	-2.7444481	5.3691931	8.4374402
C	-3.2526367	4.9832548	7.1854832
P	-0.5447356	6.5387122	4.5298681
C	1.2445273	6.5665385	4.9185907
C	1.8331314	5.3989395	5.4553244
C	3.2238064	5.3103009	5.5905385
C	4.0383251	6.3934091	5.2183584
C	3.4542096	7.5685819	4.7193578
C	2.0615015	7.6557432	4.5582936
Pd	-0.9894452	5.4462725	2.6028184
C	-0.1258369	3.7580524	3.3691026
C	-0.3400463	2.4818794	2.5583643
C	0.0331624	2.6978596	1.0879347
C	1.2875112	2.2604192	0.7951749
C	1.9649754	1.7347965	2.0583332

C	0.7639221	1.4671485	2.9959306
C	-0.9245533	3.4098169	0.2218572
C	-1.2378851	4.7573796	0.5533144
C	-2.2209071	5.4339637	-0.2123189
C	-2.8832853	4.7936631	-1.2696237
C	-2.5433878	3.4685692	-1.5978057
C	-1.5664122	2.7798469	-0.8608218
C	2.0226152	2.4439852	-0.4688536
C	1.8715021	3.6207744	-1.2409404
C	2.5731958	3.7810500	-2.4430580
C	3.4433779	2.7756189	-2.8985223
C	3.6171362	1.6107337	-2.1322607
C	2.9195436	1.4508960	-0.9266821
C	-1.7646010	1.9386419	2.7361581
O	2.8918192	2.6823721	2.5705877
O	2.2244123	5.2155510	1.7719684
C	-1.0198225	8.2662261	4.1551608
C	-0.6981421	8.7534615	2.8647302
C	-1.0706358	10.0572299	2.5035053
C	-1.7694709	10.8705457	3.4118641
C	-2.0970468	10.3808979	4.6880757
C	-1.7251295	9.0805053	5.0633018
H	2.5341751	0.7937036	1.8842039
H	1.0578538	1.5562342	4.0606254
H	0.3757008	0.4398615	2.8283312
H	0.9363617	4.0643595	3.3695485
H	-0.5214546	3.6393616	4.4000037
H	-1.9154961	1.0137102	2.1437526
H	-2.5134017	2.6860936	2.4032768
H	-1.9621843	1.7050929	3.8028531
H	2.6600901	3.5785923	2.2164507
H	1.2290304	4.4311680	-0.8729126
H	2.4486462	4.7086848	-3.0224189
H	3.9950403	2.9048457	-3.8423539
H	4.3043399	0.8217542	-2.4747774
H	3.0615959	0.5362812	-0.3315125
H	-1.3007015	1.7427493	-1.1149515
H	-3.0461345	2.9656849	-2.4384241
H	-3.6493724	5.3287385	-1.8512330
H	-2.4425215	6.4924308	0.0053926
H	-0.1875298	5.5296778	0.7547869
H	-0.1512901	8.1194593	2.1432987
H	-0.8125197	10.4339815	1.5026145
H	-2.0644672	11.8907122	3.1229928
H	-2.6479611	11.0161414	5.3981377
H	-1.9858123	8.6948915	6.0601261

H	1.2033783	4.5503061	5.7572532
H	3.6741842	4.3850168	5.9780128
H	5.1313203	6.3208134	5.3219901
H	4.0854948	8.4274347	4.4441480
H	1.6152990	8.5665729	4.1363097
H	0.0815690	7.0271287	7.4075173
H	-1.1491425	6.4011517	9.5001734
H	-3.2790055	5.0884923	9.3575619
H	-4.1830272	4.3993010	7.1223142
H	-2.9406081	5.0261264	5.0221817
C	1.8404560	6.2915201	1.2825941
O	0.7724201	6.5269049	0.5990588
O	2.5937844	7.4243112	1.4834109
H	3.3359659	7.1195772	2.0465164

S4

79

SCF Energy = -2238.396452185

C	-5.0098986	7.2424207	1.0717648
C	-4.7284723	6.7356164	2.3590208
C	-5.7493630	6.6778467	3.3313985
C	-7.0445229	7.1171545	3.0133102
C	-7.3241797	7.6204073	1.7317769
C	-6.3053407	7.6853966	0.7658101
P	-2.9957648	6.2400245	2.7100829
C	-3.1010171	5.1913415	4.2092508
C	-2.2366564	5.4024067	5.3016915
C	-2.2257790	4.4993019	6.3765723
C	-3.0743944	3.3801028	6.3700690
C	-3.9391810	3.1653581	5.2832394
C	-3.9498277	4.0613548	4.2041081
Pd	-1.6784163	5.4937382	1.0105372
C	-1.7055594	3.5597701	1.6392742
C	-0.3920004	2.8317258	1.9157319
C	0.5423330	2.8484263	0.7054267
C	0.9077666	1.5929757	0.3036580
C	0.4174773	0.5562147	1.3048366
C	-0.6814292	1.3044436	2.0871343
C	1.0827559	4.1370670	0.2342719
C	2.4910664	4.2740322	0.1672238
C	3.0877365	5.5102025	-0.1033725
C	2.2802601	6.6428502	-0.3098733
C	0.8864037	6.5139795	-0.2676741
C	0.2498318	5.2686673	-0.0040144
C	1.7234214	1.2242225	-0.8658907
C	2.5604783	0.0817984	-0.8295259

C	3.3241362	-0.2813705	-1.9485378
C	3.2654352	0.4816525	-3.1264633
C	2.4274519	1.6100047	-3.1794765
C	1.6628944	1.9764074	-2.0650678
C	0.3002606	3.4359650	3.1550822
O	1.4998191	0.0891569	2.1305778
O	-2.1386355	7.2515738	-0.4207085
C	-2.1955949	7.7878535	3.3015271
C	-0.8108232	7.9553580	3.0895529
C	-0.1640665	9.1102722	3.5554448
C	-0.8955770	10.1032864	4.2277393
C	-2.2769767	9.9415344	4.4327035
C	-2.9288300	8.7883368	3.9703985
H	0.0285983	-0.3615363	0.8173381
H	-0.7030273	0.9880633	3.1484697
H	-1.6699139	1.0609204	1.6463422
H	-2.2122729	3.1207730	0.7485008
H	-2.3648613	3.4465769	2.5202641
H	1.2106460	2.8643232	3.4299393
H	-0.3887021	3.4279825	4.0240057
H	0.5941444	4.4865496	2.9610471
H	2.0135897	0.8836821	2.3759839
H	2.6170210	-0.4989306	0.1028466
H	3.9741713	-1.1686190	-1.8983175
H	3.8650704	0.1950873	-4.0039176
H	2.3624848	2.2058538	-4.1028576
H	0.9946465	2.8478668	-2.1197447
H	-0.8633761	5.2513451	-0.8946889
H	0.2577727	7.3994847	-0.4469443
H	2.7373564	7.6244756	-0.5091089
H	4.1848752	5.5934181	-0.1386505
H	3.1163927	3.3894041	0.3592226
H	-0.2517083	7.1777800	2.5431481
H	0.9151804	9.2364884	3.3823081
H	-0.3895076	11.0122130	4.5871410
H	-2.8530635	10.7227365	4.9514545
H	-4.0120735	8.6683649	4.1209662
H	-1.5657879	6.2738500	5.3068683
H	-1.5477136	4.6731501	7.2256649
H	-3.0620687	2.6727172	7.2128050
H	-4.6054740	2.2896998	5.2712264
H	-4.6250576	3.8856508	3.3524796
H	-5.5325895	6.2878039	4.3368074
H	-7.8389720	7.0673755	3.7734892
H	-8.3408147	7.9627676	1.4854012
H	-6.5189005	8.0817689	-0.2382909

H	-4.2031643	7.2990303	0.3235752
C	-2.1313861	6.7472317	-1.5758830
O	-2.7470164	7.4533606	-2.5553734
O	-1.6027331	5.6272598	-1.9250826
H	-2.6258509	6.9325420	-3.3758587

Optimized Geometries (BXne')

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R3
79
SCF Energy = -2238.403176950
C    -1.3299944    2.9218906    2.3524434
C    -0.1375799    2.3531814    1.8507678
C     0.8888156    1.9977082    2.7477157
C     0.7207557    2.1965405    4.1278712
C    -0.4664195    2.7603493    4.6216529
C    -1.4877426    3.1321849    3.7298695
P    -0.0566067    1.9450245    0.0633459
C     1.7085071    1.4782895   -0.1839354
C     2.0319531    0.1097585   -0.0739955
C     3.3421076   -0.3338125   -0.3094203
C     4.3360241    0.5919946   -0.6694703
C     4.0189362    1.9594891   -0.7792943
C     2.7100724    2.4058144   -0.5327632
Pd   -1.3703725    0.1335633   -0.6422242
O    -0.4944093   -0.0644058   -2.9193989
C     0.8523372   -0.2031207   -3.0565548
O     1.4477346   -1.2577797   -3.0920445
C    -2.1062821   -1.7026497   -1.1388067
C    -1.7236378   -2.7575024   -0.2625694
C    -1.8767504   -4.1026399   -0.6440412
C    -2.4339327   -4.4221087   -1.8954126
C    -2.8442140   -3.3980732   -2.7607746
C    -2.6788411   -2.0458909   -2.3846153
C    -1.1695671   -2.3267556    1.0394503
C     0.0785522   -2.5126929    1.5477254
C     0.2928642   -1.6000661    2.7569170
C    -1.1188954   -1.1165736    3.1198904
C    -2.0393609   -1.3963761    1.8965634
C     1.1894815   -3.2532703    0.9176114
C     2.1044413   -3.9979022    1.7028367
C     3.1985333   -4.6484866    1.1107720
C     3.4035903   -4.5719733   -0.2771448

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C	2.4971374	-3.8458578	-1.0701619
C	1.4023623	-3.2008550	-0.4813170
C	-3.3319515	-2.1272008	2.3204636
C	-2.4192430	-0.1224472	1.1003562
O	0.9168164	-2.1806313	3.9065033
C	-0.1981128	3.5770646	-0.7664277
C	-0.6300277	3.5860500	-2.1093466
C	-0.7195664	4.7981277	-2.8100672
C	-0.3908199	6.0070450	-2.1730747
C	0.0303708	6.0027340	-0.8323503
C	0.1292339	4.7918262	-0.1287010
O	1.3882439	1.0242292	-3.1529083
H	2.3596438	0.9147794	-3.0753877
H	0.9178374	-0.7402168	2.4089996
H	-1.1297559	-0.0556263	3.4342990
H	-1.4445917	-1.7245618	3.9882384
H	-2.2585051	0.7864030	1.7079084
H	-3.4756271	-0.1511307	0.7688042
H	-3.0976227	-3.0598606	2.8738620
H	-3.9408188	-2.3950657	1.4333238
H	-3.9465373	-1.4775007	2.9778188
H	1.8742134	-2.2017515	3.7255339
H	1.9234669	-4.0878126	2.7834215
H	3.8923971	-5.2278725	1.7395749
H	4.2641110	-5.0794704	-0.7394631
H	2.6439153	-3.7576895	-2.1567785
H	0.7229287	-2.6177719	-1.1152195
H	-1.5520665	-4.8993926	0.0427892
H	-2.5548591	-5.4758850	-2.1891912
H	-3.3034364	-3.6446645	-3.7311265
H	-3.0325444	-1.2569853	-3.0715788
H	-0.9021824	-0.9751675	-2.8922401
H	-0.8936697	2.6361725	-2.5985432
H	-1.0561848	4.7993866	-3.8577887
H	-0.4690500	6.9579007	-2.7218569
H	0.2835752	6.9489172	-0.3301322
H	0.4563969	4.7870221	0.9220154
H	1.2350192	-0.6135228	0.1576091
H	3.5669564	-1.4079491	-0.2386591
H	5.3619599	0.2477068	-0.8705570
H	4.7976643	2.6845032	-1.0621850
H	2.4600022	3.4719166	-0.6367424
H	1.8224159	1.5615178	2.3642878
H	1.5233802	1.9038162	4.8211273
H	-0.5976775	2.9103338	5.7037424
H	-2.4195181	3.5767507	4.1107727

H	-2.1358810	3.2040530	1.6567498
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R4

79

SCF Energy = -2238.419766294

C	1.4122567	2.5902602	2.6046786
C	0.1535446	2.2134880	2.0818836
C	-0.9248817	1.9987569	2.9631705
C	-0.7425112	2.1472802	4.3481844
C	0.5080565	2.5240960	4.8611107
C	1.5846813	2.7525922	3.9857640
P	0.0542601	1.9705128	0.2649856
C	-1.6415032	1.3283658	-0.0461005
C	-2.5021203	1.9496957	-0.9721482
C	-3.7048543	1.3236203	-1.3427321
C	-4.0613269	0.0872442	-0.7808192
C	-3.2120615	-0.5287327	0.1550777
C	-2.0020391	0.0792033	0.5128647
Pd	1.3290421	0.2542975	-0.7359889
C	2.3421218	-0.2565210	0.9723072
C	2.5198380	-1.7534502	1.3356123
C	1.4131858	-2.5335304	0.6116352
C	0.3463781	-2.7997477	1.4249362
C	0.6456033	-2.3009930	2.8418585
C	2.1636681	-2.0402247	2.8184338
C	-0.9928331	-3.3038926	1.0753717
C	-1.9910248	-3.4096795	2.0796509
C	-3.2808723	-3.8730430	1.7819367
C	-3.6225209	-4.2353402	0.4683220
C	-2.6540124	-4.1177098	-0.5437734
C	-1.3633691	-3.6637379	-0.2465919
C	1.6432935	-2.7040722	-0.8370461
C	1.7794366	-3.9688044	-1.4488124
C	2.1382912	-4.0602636	-2.8024916
C	2.3610341	-2.8893555	-3.5479468
C	2.2121030	-1.6278930	-2.9431190
C	1.8659029	-1.5120342	-1.5787054
D	-0.1410760	-1.1511612	3.2039144
C	3.9293169	-2.2388696	0.9680123
D	-1.0544101	-1.0244919	-2.3647959
C	0.0157178	3.6885858	-0.3855014
C	-0.4992239	4.7589279	0.3754417
C	-0.5305520	6.0528925	-0.1658633
C	-0.0535181	6.2847521	-1.4678323
C	0.4576790	5.2198502	-2.2282377
C	0.4991021	3.9238207	-1.6897335

H	0.3769535	-3.0597011	3.6063421
H	2.6947510	-2.9587572	3.1436534
H	2.4496751	-1.2254124	3.5139746
H	1.8038895	0.2576578	1.7919382
H	3.3222282	0.2554239	0.8489776
H	4.6846504	-1.7394286	1.6090908
H	4.1641278	-2.0031160	-0.0885884
H	4.0276878	-3.3355981	1.1045145
H	0.2150516	-0.3809221	2.7183619
H	-0.6270805	-3.5886162	-1.0557500
H	-2.9046539	-4.3840444	-1.5820698
H	-4.6348421	-4.5982468	0.2344307
H	-4.0293694	-3.9430396	2.5862238
H	-1.7627950	-3.0908611	3.1047863
H	-0.3406405	-1.1998009	-1.6791231
H	2.3658063	-0.7185661	-3.5457744
H	2.6530753	-2.9589450	-4.6078630
H	2.2514476	-5.0480262	-3.2749769
H	1.6069247	-4.8792372	-0.8536949
H	-2.2215618	2.9136299	-1.4209035
H	-4.3665979	1.8129274	-2.0740357
H	-5.0031298	-0.4025484	-1.0721116
H	-3.4744497	-1.5016157	0.5939068
H	-1.3404487	-0.4337061	1.2273156
H	-0.8725185	4.5761998	1.3943430
H	-0.9300872	6.8859587	0.4324101
H	-0.0784225	7.3010875	-1.8897077
H	0.8325273	5.3982887	-3.2474461
H	0.8891299	3.0830834	-2.2818500
H	-1.9063450	1.7010378	2.5679998
H	-1.5865847	1.9621712	5.0289630
H	0.6482651	2.6339462	5.9469687
H	2.5680905	3.0458797	4.3829735
H	2.2586755	2.7519344	1.9186584
C	-0.7454246	0.1244189	-2.9521647
O	0.2193453	0.8402467	-2.6734096
O	-1.5934596	0.4656891	-3.9265666
H	-2.3095069	-0.2028614	-3.9453276

S3

79

SCF Energy = -2238.411308685

C	-0.3658341	-2.4395423	3.6915636
C	0.3791844	-1.2428446	3.6560674
C	1.4157869	-1.0348627	4.5905208
C	1.6943304	-2.0139172	5.5559767

C	0.9435373	-3.2023504	5.5934238
C	-0.0859356	-3.4149236	4.6615003
P	-0.0579837	-0.0019246	2.3825266
C	1.5365536	0.8113490	1.9748742
C	2.6182502	-0.0098756	1.5866673
C	3.7902282	0.5620667	1.0761267
C	3.8996445	1.9576009	0.9575260
C	2.8350945	2.7787043	1.3610511
C	1.6545482	2.2107731	1.8667109
Pd	-1.2005961	-0.7037452	0.4431769
C	0.3597568	-1.8527318	-0.2237451
C	0.1716298	-2.6267074	-1.5261358
C	-0.2781187	-1.6332170	-2.6014773
C	0.7611706	-1.2134730	-3.3842924
C	2.0539310	-1.9294001	-2.9922948
C	1.5630920	-3.0689463	-2.0703933
C	-1.6763151	-1.1775790	-2.5489201
C	-2.2318882	-0.8868732	-1.2755419
C	-3.5744227	-0.4602213	-1.1968932
C	-4.3657893	-0.3414261	-2.3553565
C	-3.8118295	-0.6434855	-3.6113210
C	-2.4757636	-1.0576548	-3.7074783
C	0.8106520	-0.0717256	-4.3175032
C	-0.0456111	1.0488515	-4.1746950
C	0.0751527	2.1641227	-5.0123383
C	1.0500455	2.1902134	-6.0256638
C	1.9096931	1.0903119	-6.1800109
C	1.7965913	-0.0208375	-5.3321131
C	-0.7803023	-3.8170963	-1.3434416
O	2.9911164	-1.0487723	-2.3832744
O	1.6240949	1.0988787	-1.3192383
C	-1.0477347	1.2734948	3.2572290
C	-1.6997569	2.2464556	2.4640382
C	-2.4956494	3.2300091	3.0701099
C	-2.6618522	3.2409792	4.4655614
C	-2.0256022	2.2681193	5.2543768
C	-1.2187926	1.2872502	4.6557736
H	2.5731048	-2.3642090	-3.8769636
H	2.3074365	-3.2787615	-1.2769757
H	1.4251901	-3.9983444	-2.6615525
H	1.1702967	-1.1055069	-0.3193582
H	0.5345536	-2.5302196	0.6415339
H	-0.9477377	-4.3423239	-2.3053510
H	-1.7629574	-3.4809170	-0.9578037
H	-0.3536456	-4.5435123	-0.6209509
H	2.4961924	-0.2824432	-2.0126238

H	-0.8004592	1.0529110	-3.3784470
H	-0.5933028	3.0257459	-4.8634655
H	1.1439588	3.0663798	-6.6853864
H	2.6829901	1.1001501	-6.9636260
H	2.4907900	-0.8646918	-5.4518372
H	-2.0339039	-1.2895825	-4.6886029
H	-4.4267491	-0.5601781	-4.5204482
H	-5.4169286	-0.0230354	-2.2741695
H	-4.0265598	-0.2189461	-0.2176673
H	-0.6223104	1.0106445	-0.5874061
H	-1.5718557	2.2425141	1.3693688
H	-2.9931314	3.9873579	2.4458677
H	-3.2932863	4.0077588	4.9392433
H	-2.1577770	2.2711742	6.3470155
H	-0.7241544	0.5258411	5.2765645
H	2.5383486	-1.1035923	1.6700239
H	4.6135142	-0.0892699	0.7484775
H	4.8177296	2.4040907	0.5468125
H	2.9157540	3.8730434	1.2774720
H	0.8207580	2.8609296	2.1676142
H	2.0078539	-0.1078797	4.5521080
H	2.5042484	-1.8502997	6.2830025
H	1.1679659	-3.9698951	6.3495569
H	-0.6683147	-4.3482418	4.6837202
H	-1.1601059	-2.6006836	2.9444018
C	0.8292849	2.0279456	-1.2917195
O	-0.4296172	1.9744821	-0.8685099
O	1.1259076	3.2795006	-1.6914092
H	2.0442609	3.2281303	-2.0271394

S4

79

SCF Energy = -2238.409022733

C	-0.4812136	3.9118792	-2.0798671
C	-0.9533640	3.5021043	-0.8125591
C	-2.2377890	3.9000463	-0.3910353
C	-3.0416060	4.6910350	-1.2293153
C	-2.5710101	5.0896110	-2.4903442
C	-1.2867853	4.7010174	-2.9109837
P	0.1238374	2.3773013	0.1690381
C	-0.6753187	2.3242377	1.8218109
C	-0.1439918	2.9669210	2.9557976
C	-0.7722101	2.8252181	4.2046749
C	-1.9344208	2.0480057	4.3290023
C	-2.4680218	1.4015760	3.1999780
C	-1.8357272	1.5288609	1.9555945

Pd	0.5670354	0.2239421	-0.7237280
C	0.8388641	-0.4654915	1.1763552
C	1.5461328	-1.7986538	1.4310178
C	0.8499656	-2.9006645	0.6390888
C	0.2888282	-3.8534037	1.4480993
C	0.7683039	-3.6782695	2.8807018
C	1.3071335	-2.2320336	2.9162037
C	0.9260115	-2.8595636	-0.8296233
C	1.1246347	-4.0691610	-1.5422852
C	1.3220441	-4.0704653	-2.9265311
C	1.3336851	-2.8499389	-3.6219098
C	1.1339525	-1.6455920	-2.9259032
C	0.9238085	-1.6179949	-1.5256554
C	-0.6157550	-4.9548696	1.0738983
C	-0.5800723	-6.1892280	1.7678617
C	-1.4696983	-7.2228302	1.4379172
C	-2.4154390	-7.0467601	0.4147127
C	-2.4703190	-5.8203267	-0.2726550
C	-1.5851128	-4.7862549	0.0541766
C	3.0452193	-1.7014778	1.0873452
O	1.7618902	-4.6685290	3.2107541
O	-0.1308808	1.0722490	-2.8149385
C	1.6451655	3.3739116	0.4166776
C	2.8859744	2.7040748	0.4321129
C	4.0719871	3.4259732	0.6407643
C	4.0245779	4.8173652	0.8266922
C	2.7897427	5.4901278	0.8008939
C	1.6018218	4.7729775	0.5954719
H	-0.0377042	-3.8433566	3.6257035
H	2.2291660	-2.1816145	3.5284745
H	0.5608532	-1.5648073	3.3934240
H	-0.2004016	-0.5203542	1.5636831
H	1.3613569	0.3413160	1.7379580
H	3.5701315	-2.6544927	1.3043841
H	3.5270478	-0.9023842	1.6883108
H	3.1866707	-1.4647363	0.0143807
H	2.3545736	-4.7159819	2.4345576
H	0.1740972	-6.3240866	2.5571693
H	-1.4207928	-8.1772438	1.9848741
H	-3.1120622	-7.8588837	0.1560844
H	-3.2166575	-5.6672474	-1.0675714
H	-1.6383474	-3.8248962	-0.4772615
H	-1.4027034	-0.1455643	-1.3376361
H	1.1478054	-0.7026847	-3.4923343
H	1.5078975	-2.8309426	-4.7095948
H	1.4841542	-5.0201979	-3.4590364

H	1.1426601	-5.0171131	-0.9844372
H	2.9116003	1.6148542	0.2672091
H	5.0377710	2.8988275	0.6492639
H	4.9550446	5.3835383	0.9849584
H	2.7532669	6.5815311	0.9383426
H	0.6348047	5.2979803	0.5658074
H	0.7687814	3.5733250	2.8647905
H	-0.3457803	3.3252013	5.0874854
H	-2.4223562	1.9372231	5.3090723
H	-3.3726016	0.7818694	3.2925373
H	-2.2361820	0.9979224	1.0775258
H	-2.6105469	3.5980996	0.5982132
H	-4.0416097	5.0001094	-0.8887058
H	-3.2034482	5.7065461	-3.1466121
H	-0.9116518	5.0074949	-3.8987852
H	0.5156044	3.5969328	-2.4203165
C	-1.3387624	0.8599981	-2.9213541
O	-2.0369746	1.3307492	-3.9586826
O	-2.0729406	0.1659457	-2.0510351
H	-2.9713049	1.0599234	-3.8453408

Optimized Geometries (BXnj)

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R3
73
SCF Energy = -1973.528249972
C    -0.3054954   -1.4253055   -1.7866323
C    -0.3352563   -2.7089766   -1.1786563
C    -0.7453731   -3.8191581   -1.9633185
C    -1.0632127   -3.6753859   -3.3188511
C    -0.9799352   -2.4137624   -3.9330581
C    -0.6014875   -1.3016893   -3.1612689
C     0.0358547   -2.8621786    0.2383185
C     0.4283547   -3.9936271    0.8970822
C     0.6651318   -5.3487278    0.3563099
C    -0.1167933   -6.4477397    0.7838475
C     0.1372304   -7.7423479    0.3030512
C     1.1763259   -7.9626570   -0.6152706
C     1.9599379   -6.8786672   -1.0493187
C     1.7100159   -5.5869355   -0.5665899
C    -0.0508862   -1.6660868    1.1921108
C    -1.5271015   -1.3474744    1.5135241
C     0.6919336   -0.4443924    0.6643151

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C	0.6780366	-2.2033356	2.4636774
C	0.5993754	-3.7334241	2.3902986
O	-0.5242360	-4.1983329	3.1622580
H	1.5304334	-4.2115944	2.7764425
H	1.7447092	-1.9010339	2.4386757
H	0.2368886	-1.8198120	3.4041674
H	1.7348967	-0.7026122	0.3830772
H	0.6990768	0.3590353	1.4302689
H	-2.0020420	-2.2167816	2.0087195
H	-2.0836822	-1.1050174	0.5863564
H	-1.5940394	-0.4713000	2.1898832
H	-0.4452652	-5.1689035	3.2146852
H	-0.9618992	-6.2685182	1.4660265
H	-0.4895253	-8.5826675	0.6395495
H	1.3734320	-8.9763303	-0.9959061
H	2.7750907	-7.0430775	-1.7708099
H	2.3187505	-4.7358104	-0.9065751
H	-0.8322362	-4.8083791	-1.4949755
H	-1.3799557	-4.5546904	-3.9003514
H	-1.2164994	-2.2944168	-5.0021388
H	-0.5522668	-0.3096235	-3.6509336
Pd	-0.1309467	0.4076336	-1.0006948
P	-0.2063240	2.5790984	-0.1412538
C	-1.1022904	3.8595067	-1.1119352
C	-0.9159156	3.8524329	-2.5107604
H	-0.2734243	3.0821685	-2.9682593
C	-1.5410691	4.8178340	-3.3135102
H	-1.3897573	4.8052792	-4.4034385
C	-2.3663078	5.7922726	-2.7262136
H	-2.8631816	6.5455698	-3.3560933
C	-2.5621360	5.7989158	-1.3350529
H	-3.2114455	6.5582493	-0.8731843
C	-1.9328041	4.8377863	-0.5277458
H	-2.0949845	4.8395392	0.5605813
C	1.3972404	3.3949647	0.2472730
C	2.5807506	2.6433754	0.1072474
H	2.5137314	1.6034196	-0.2488729
C	3.8233489	3.2230941	0.4124400
H	4.7445470	2.6313581	0.3016176
C	3.8883924	4.5551601	0.8514102
H	4.8622202	5.0105057	1.0875267
C	2.7094841	5.3114175	0.9831782
H	2.7602092	6.3580261	1.3200487
C	1.4671698	4.7353997	0.6815428
H	0.5462431	5.3303479	0.7782986
C	-1.0825117	2.5345208	1.4715395

C	-0.3984202	2.6527617	2.6972420
H	0.6721216	2.9050473	2.7056865
C	-1.0812253	2.4445933	3.9082059
H	-0.5373887	2.5320462	4.8609642
C	-2.4479884	2.1272765	3.9040293
H	-2.9799523	1.9637218	4.8532375
C	-3.1345952	2.0087079	2.6818735
H	-4.2036996	1.7486685	2.6717734
C	-2.4544269	2.1973378	1.4719983
H	-2.9857546	2.0677401	0.5163143

R4

73

SCF Energy = -1973.530119062

C	-0.1631768	-6.5363439	1.0223010
C	-0.5496771	-5.3444599	0.3630169
C	-1.3820764	-5.4530452	-0.7786598
C	-1.7783873	-6.7046252	-1.2646881
C	-1.3630804	-7.8815034	-0.6152388
C	-0.5586063	-7.7898335	0.5322709
C	-0.1638528	-4.0273747	0.8987417
Pd	0.1514143	0.3970481	-0.9936941
P	0.1591759	2.5736515	-0.1415254
C	0.1914327	-2.8834409	0.2318088
C	0.5141258	-2.7027571	-1.1930015
C	0.9921851	-3.7811820	-1.9830025
C	1.2801900	-3.6154780	-3.3416930
C	1.0967478	-2.3618545	-3.9531837
C	0.6577694	-1.2780486	-3.1740036
C	0.3993507	-1.4213032	-1.7928674
C	-0.1606777	-3.7916464	2.4087958
O	-1.1329789	-4.5217317	3.1418879
C	-0.2990939	-2.2588565	2.5054515
C	0.3217259	-1.6939046	1.1919470
C	-0.4969553	-0.4935644	0.7269396
C	1.8028417	-1.3170563	1.4059493
H	0.8149649	-4.1197103	2.8386039
H	0.1567476	-1.8255425	3.4173549
H	-1.3869793	-2.0351002	2.5356905
H	-1.5486470	-0.7885427	0.5262676
H	-0.4733493	0.3046947	1.4982809
H	1.8891279	-0.4495957	2.0910494
H	2.2708064	-1.0364186	0.4414458
H	2.3721548	-2.1650343	1.8383781
H	-1.9598847	-4.4840330	2.6230353
H	-1.7144959	-4.5338007	-1.2828688

H	-2.4232212	-6.7637966	-2.1550082
H	-1.6757134	-8.8655171	-0.9966110
H	-0.2383301	-8.7041589	1.0551699
H	0.4546319	-6.4757007	1.9292269
H	0.5369436	-0.2908388	-3.6609655
H	1.3083216	-2.2260468	-5.0254850
H	1.6515926	-4.4689978	-3.9291844
H	1.1480323	-4.7620444	-1.5126743
C	0.9413399	3.8859289	-1.1658883
C	1.1239022	2.5820984	1.4212314
C	-1.4574338	3.3147686	0.3315205
C	-1.5724500	4.6614049	0.7358489
C	-2.8218192	5.1777713	1.1083360
C	-3.9627648	4.3554293	1.0777280
C	-3.8533746	3.0166853	0.6686818
C	-2.6039908	2.4966305	0.2923621
H	-0.6817455	5.3077542	0.7534914
H	-2.9080597	6.2293944	1.4214583
H	-4.9422674	4.7640809	1.3691847
H	-4.7454619	2.3731481	0.6366621
H	-2.5040752	1.4522396	-0.0422811
C	1.7599949	4.9026157	-0.6326738
C	2.3019856	5.8843443	-1.4777411
C	2.0301044	5.8600677	-2.8558213
C	1.2161369	4.8475532	-3.3923631
C	0.6782013	3.8617255	-2.5521731
H	1.9812753	4.9188248	0.4450669
H	2.9425372	6.6737063	-1.0557812
H	2.4586734	6.6295855	-3.5155297
H	1.0055210	4.8214959	-4.4721461
H	0.0448999	3.0620626	-2.9703591
C	0.5069734	2.6996381	2.6820433
C	1.2646491	2.5376800	3.8550570
C	2.6393262	2.2672420	3.7773182
C	3.2589227	2.1491480	2.5196295
C	2.5045968	2.2919123	1.3479446
H	-0.5695831	2.9152396	2.7477656
H	0.7733833	2.6248559	4.8359670
H	3.2303105	2.1412110	4.6969318
H	4.3345690	1.9271798	2.4522927
H	2.9845953	2.1640303	0.3652277

S3

73

SCF Energy = -1973.536049086

C	-2.4039375	-1.5754531	-0.8978165
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C	-1.7977654	-2.7055801	-0.2856861
C	-2.1179838	-4.0096014	-0.7133856
C	-3.0590257	-4.1967073	-1.7393627
C	-3.6736532	-3.0855193	-2.3417208
C	-3.3479054	-1.7794502	-1.9233288
C	-0.8366261	-2.4069452	0.7954743
C	0.4756829	-2.7507109	0.9292828
C	1.3345355	-3.4676271	-0.0256490
C	1.1025569	-3.4130678	-1.4236552
C	1.9861832	-4.0189721	-2.3242312
C	3.1324810	-4.6910061	-1.8603887
C	3.3803276	-4.7544898	-0.4801306
C	2.4934381	-4.1509001	0.4256291
C	-1.3287380	-1.5301923	1.9547032
C	-2.2476771	-2.3712911	2.8725125
C	-2.1017421	-0.3011162	1.4387229
C	-0.0035496	-1.1514105	2.6652538
C	1.0675199	-2.1561238	2.2070932
O	2.2988717	-1.4563885	2.0017912
H	1.2226089	-2.9635839	2.9690451
H	0.3366988	-0.1608874	2.3136992
H	-0.1103932	-1.0920787	3.7659437
H	-1.8698277	0.6109413	2.0240987
H	-3.1954908	-0.4651771	1.4191775
H	-1.6973678	-3.2347506	3.3002205
H	-3.1148976	-2.7642214	2.3041668
H	-2.6317795	-1.7543808	3.7111557
H	2.8530409	-2.0082869	1.4151133
H	0.2273905	-2.8669010	-1.8004891
H	1.7858100	-3.9536810	-3.4045862
H	3.8283540	-5.1599867	-2.5721840
H	4.2697846	-5.2814836	-0.1020524
H	2.6931782	-4.2288542	1.5059075
H	-1.6240683	-4.8728839	-0.2409542
H	-3.3195189	-5.2152099	-2.0657645
H	-4.4196140	-3.2349162	-3.1385307
H	-3.8394066	-0.9198358	-2.4078471
Pd	-1.5364515	0.1888054	-0.4843084
P	0.0039739	1.9439389	-0.1429828
C	-0.2315350	3.5879993	-0.9344204
C	-0.9271313	3.6272808	-2.1608507
H	-1.3364722	2.6941200	-2.5814358
C	-1.1046435	4.8438327	-2.8361825
H	-1.6480991	4.8653327	-3.7928966
C	-0.5993296	6.0336925	-2.2843245
H	-0.7448392	6.9896883	-2.8098166

C	0.0838724	6.0026762	-1.0569979
H	0.4758218	6.9339127	-0.6202461
C	0.2699268	4.7851363	-0.3826982
H	0.8012634	4.7615822	0.5806859
C	1.6345334	1.3798964	-0.7867555
C	1.8594092	-0.0110636	-0.8522472
H	1.0553932	-0.6987451	-0.5470024
C	3.0951986	-0.5070691	-1.2955995
H	3.2548994	-1.5944658	-1.3475371
C	4.1096675	0.3850167	-1.6782966
H	5.0784751	-0.0018962	-2.0296816
C	3.8869997	1.7731336	-1.6226174
H	4.6798822	2.4718851	-1.9303710
C	2.6530164	2.2726538	-1.1794922
H	2.4778843	3.3584268	-1.1429892
C	0.3516577	2.3641848	1.6088602
C	1.5605743	2.0110396	2.2396119
H	2.3526608	1.5072913	1.6686424
C	1.7332750	2.2586339	3.6113005
H	2.6760131	1.9676461	4.0981964
C	0.7069999	2.8576454	4.3584446
H	0.8449223	3.0467141	5.4338045
C	-0.5034518	3.2063918	3.7326135
H	-1.3138469	3.6700021	4.3153866
C	-0.6852903	2.9539393	2.3656439
H	-1.6370342	3.2175388	1.8771571

S4

73

SCF Energy = -1973.533273633

C	3.8348029	1.0954248	-1.9169227
C	2.7627198	0.6563887	-1.0975146
C	1.4464874	0.6727738	-1.6252521
C	1.2475043	1.0551612	-2.9696373
C	2.3199009	1.4628852	-3.7813251
C	3.6183036	1.4932497	-3.2406238
C	2.9889795	0.2416002	0.2955506
C	4.1124141	-0.3091762	0.8585152
C	5.3231160	-0.8351298	0.2015926
C	6.5974464	-0.6567966	0.7930636
C	7.7467216	-1.1940946	0.1935939
C	7.6479023	-1.9268144	-1.0004071
C	6.3849663	-2.1271869	-1.5871883
C	5.2359588	-1.5916128	-0.9929047
C	1.8821002	0.4685201	1.3295174
C	1.6116450	1.9717523	1.5460750

C	0.6016058	-0.2702901	0.9397960
C	2.4801415	-0.1936991	2.6137381
C	3.9987446	-0.2990766	2.3758237
O	4.7540302	0.7886769	2.9422743
H	4.4310513	-1.2075421	2.8440014
H	2.2533776	0.3760119	3.5363486
H	2.0649491	-1.2148450	2.7396879
H	0.8109179	-1.3492179	0.7741331
H	-0.1654450	-0.1504407	1.7334741
H	2.5139057	2.4869602	1.9346459
H	0.7940807	2.1143136	2.2818052
H	1.3117090	2.4547269	0.5951633
H	4.5975656	1.5551119	2.3560217
H	6.6664274	-0.0767945	1.7253166
H	8.7295196	-1.0375612	0.6647012
H	8.5500734	-2.3479557	-1.4698013
H	6.2948373	-2.7139046	-2.5144145
H	4.2489596	-1.7595141	-1.4480126
H	0.2275985	1.0540657	-3.4014607
H	2.1417811	1.7687917	-4.8242148
H	4.4658359	1.8333473	-3.8550029
H	4.8504098	1.1309992	-1.4975143
Pd	-0.3310424	0.3133333	-0.7802959
P	-2.5294905	0.1114647	0.0066607
C	-2.7604520	0.8944587	1.6531282
C	-3.4869774	0.2960683	2.7006390
H	-3.9659682	-0.6821142	2.5468269
C	-3.5934586	0.9468903	3.9415167
H	-4.1576127	0.4723850	4.7587630
C	-2.9816801	2.1951201	4.1403900
H	-3.0649156	2.7004816	5.1144495
C	-2.2538818	2.7943229	3.0966523
H	-1.7648039	3.7679913	3.2507420
C	-2.1349632	2.1434931	1.8609100
H	-1.5411757	2.5903688	1.0476522
C	-3.2454819	-1.5693480	0.2157167
C	-4.6262781	-1.8233846	0.0832037
H	-5.3107834	-1.0032165	-0.1814264
C	-5.1235728	-3.1208866	0.2824636
H	-6.2015125	-3.3153562	0.1744144
C	-4.2484763	-4.1687595	0.6161210
H	-4.6408744	-5.1854921	0.7695634
C	-2.8713301	-3.9198665	0.7442442
H	-2.1822641	-4.7400874	0.9959596
C	-2.3687391	-2.6260318	0.5385727
H	-1.2893703	-2.4270845	0.6193914

C	-3.7623585	0.9606730	-1.0615244
C	-4.7402686	1.8430311	-0.5616187
H	-4.7917774	2.0467544	0.5182449
C	-5.6432189	2.4620074	-1.4420735
H	-6.4035854	3.1523106	-1.0461650
C	-5.5781548	2.2024652	-2.8207295
H	-6.2860572	2.6905530	-3.5075008
C	-4.6034682	1.3224282	-3.3236722
H	-4.5464763	1.1192699	-4.4037211
C	-3.6957445	0.7083302	-2.4494521
H	-2.9276027	0.0217535	-2.8424444

Optimized Geometries (TS-BXnj/k-f')

R3
73
SCF Energy = -1973.505963658

C	1.7104604	5.2455665	1.0463054
C	1.1751045	4.1423223	0.3112805
C	1.1788440	4.2156447	-1.1033723
C	1.7349499	5.3181418	-1.7657742
C	2.3414010	6.3562209	-1.0364745
C	2.3596329	6.3052151	0.3697906
C	0.9075071	2.9388779	1.0987185
C	0.7115500	1.6234426	0.7652167
C	0.2306535	1.0391020	-0.4964604
C	-0.8707072	1.6111495	-1.1822639
C	-1.3589343	1.0430221	-2.3663285
C	-0.7667647	-0.1199994	-2.8897131
C	0.3124871	-0.7123478	-2.2122779
C	0.8013485	-0.1443271	-1.0271090
C	1.1405666	3.0936490	2.6054397
C	-0.2182265	3.3414945	3.3059121
C	2.1072054	4.2485797	2.8357881
C	1.6642667	1.6804569	2.9779568
C	0.9743677	0.7317712	1.9772253
O	-0.2368714	0.2070570	2.5434992
H	1.6453664	-0.1198701	1.7044573
H	2.7607816	1.6326621	2.8175781
H	1.4511511	1.3895051	4.0251299
H	3.1244376	4.0516067	2.4507562
H	2.1882544	4.5547115	3.9015008
H	-0.8682902	2.4545594	3.1851693

H	-0.7227454	4.2345057	2.8802680
H	-0.0694729	3.5284358	4.3889652
H	-0.7925999	-0.0750094	1.7916947
H	-1.3465893	2.5084528	-0.7588061
H	-2.2154656	1.5052114	-2.8806468
H	-1.1509892	-0.5678690	-3.8185985
H	0.7807914	-1.6242305	-2.6133811
H	1.6544055	-0.6098034	-0.5107959
H	0.7753884	3.3808654	-1.6916390
H	1.7283302	5.3490556	-2.8659625
H	2.8128048	7.2025961	-1.5599004
H	2.8686499	7.1000853	0.9376291
Pd	0.9696346	6.1464869	2.6981212
P	-0.0415154	7.3117795	4.3886940
C	-1.2238129	8.6450587	3.9163347
C	-0.9551403	9.3560922	2.7282318
H	-0.0878658	9.0638082	2.1135238
C	-1.7902560	10.4105834	2.3292403
H	-1.5732411	10.9592562	1.4002209
C	-2.9088191	10.7545220	3.1074235
H	-3.5691720	11.5761054	2.7906749
C	-3.1904176	10.0399741	4.2842240
H	-4.0715858	10.3006025	4.8903124
C	-2.3522528	8.9890756	4.6895903
H	-2.5840787	8.4205686	5.6029745
C	1.0782628	8.1516114	5.5924096
C	2.4530668	7.8481851	5.5331802
H	2.8049394	7.1520369	4.7535531
C	3.3472466	8.4322003	6.4454225
H	4.4196037	8.1898987	6.3930898
C	2.8726382	9.3287530	7.4164787
H	3.5724873	9.7912116	8.1291839
C	1.5025989	9.6418155	7.4736166
H	1.1299550	10.3498719	8.2295431
C	0.6074675	9.0565303	6.5660415
H	-0.4623389	9.3096894	6.6104731
C	-1.0507772	6.2058392	5.4575169
C	-0.5934805	5.7720728	6.7177824
H	0.3341070	6.1897239	7.1365199
C	-1.3161687	4.8050119	7.4365558
H	-0.9489552	4.4705982	8.4188681
C	-2.5004682	4.2678053	6.9076356
H	-3.0636431	3.5089401	7.4713786
C	-2.9618266	4.6999498	5.6511668
H	-3.8864983	4.2792152	5.2279199
C	-2.2386850	5.6561550	4.9262902

H	-2.5911527	5.9757302	3.9332311
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R4

73

SCF Energy = -1973.504814435

C	4.1058588	0.9459690	0.0030686
C	2.6950536	0.8994279	-0.0959248
C	2.1119739	-0.1419531	-0.8568485
C	2.9113831	-1.0782279	-1.5271818
C	4.3124213	-1.0005138	-1.4445880
C	4.9048731	0.0126580	-0.6721986
C	1.8632107	1.8576020	0.6555806
Pd	-2.0443071	4.8816221	-0.0498971
P	-2.6796254	7.0111992	0.4702556
C	0.7605614	2.5713513	0.2752777
C	-0.0437358	2.6266476	-0.9436089
C	0.3353883	2.1345434	-2.2140465
C	-0.6067164	2.0164219	-3.2458374
C	-1.9558318	2.3387225	-3.0151002
C	-2.3518706	2.8605059	-1.7673215
C	-1.3776256	3.1039349	-0.7687368
C	2.1361924	2.0863634	2.1500705
O	2.6704146	0.9662285	2.8323130
C	0.7580435	2.5704216	2.6612476
C	0.1608666	3.3414059	1.4555615
C	-1.3570761	3.2786579	1.3172829
C	0.6707134	4.8010856	1.4677518
H	2.8988485	2.8875528	2.2904857
H	0.8177824	3.1733238	3.5890996
H	0.1466990	1.6666049	2.8729439
H	-1.7519347	2.2489873	1.3912701
H	-1.8979467	3.9182950	2.0497845
H	0.2129647	5.3744685	2.2987447
H	0.3999379	5.3155603	0.5220557
H	1.7726505	4.8393448	1.5826759
H	2.1536199	0.1881903	2.5455957
H	1.0157312	-0.2155742	-0.9092206
H	2.4362627	-1.8803625	-2.1126676
H	4.9404280	-1.7350978	-1.9711514
H	6.0009306	0.0733744	-0.5903865
H	4.5768195	1.7284275	0.6156053
H	-3.4124377	3.1000150	-1.5897429
H	-2.7057833	2.1930493	-3.8081589
H	-0.2921461	1.6335892	-4.2285604
H	1.3750926	1.8219410	-2.3822498
C	-2.8676658	8.2139579	-0.9141043

C	-1.4336102	7.8120377	1.5627151
C	-4.2525110	7.2078331	1.4166455
C	-4.8605914	8.4618665	1.6308062
C	-6.0385682	8.5524459	2.3869843
C	-6.6178526	7.3937894	2.9347184
C	-6.0193132	6.1417961	2.7194911
C	-4.8423110	6.0485431	1.9587961
H	-4.4151981	9.3703249	1.1988474
H	-6.5104483	9.5337496	2.5482796
H	-7.5430948	7.4685276	3.5262489
H	-6.4734853	5.2316994	3.1399705
H	-4.3637622	5.0742966	1.7645563
C	-2.5991184	9.5926189	-0.7830778
C	-2.7964702	10.4556292	-1.8727376
C	-3.2635174	9.9507742	-3.0981423
C	-3.5249795	8.5769271	-3.2362449
C	-3.3213973	7.7110990	-2.1511490
H	-2.2178800	9.9885392	0.1704945
H	-2.5807737	11.5296649	-1.7648502
H	-3.4146231	10.6292537	-3.9514980
H	-3.8783917	8.1755090	-4.1981133
H	-3.5009143	6.6284489	-2.2554442
C	-1.6402928	7.9465846	2.9501187
C	-0.6054113	8.4168533	3.7760222
C	0.6393199	8.7613756	3.2254479
C	0.8487580	8.6318502	1.8405320
C	-0.1768619	8.1529947	1.0147591
H	-2.6140661	7.6788550	3.3864660
H	-0.7765060	8.5162064	4.8588576
H	1.4483993	9.1291911	3.8743190
H	1.8228295	8.8970407	1.4020900
H	-0.0021427	8.0328221	-0.0658584

S3

73

SCF Energy = -1973.521566115

C	-2.1964700	4.3705534	0.5641955
C	-1.2156984	3.3987756	0.2045706
C	-1.0357028	3.0505759	-1.1476195
C	-1.8467356	3.6441602	-2.1302520
C	-2.8402320	4.5743399	-1.7714714
C	-3.0301028	4.9337890	-0.4230187
C	-0.5904203	2.8053221	1.3935250
C	0.6759703	2.4973839	1.7929595
C	1.9356714	2.6358684	1.0506766
C	2.0814813	3.5657169	-0.0105721

C	3.3087913	3.7302168	-0.6621182
C	4.4327078	2.9777179	-0.2720653
C	4.3097345	2.0550991	0.7787372
C	3.0789353	1.8858658	1.4323228
C	-1.6291699	2.5527802	2.4930087
C	-2.3404845	1.2083079	2.2205192
C	-2.6489875	3.7064635	2.4556269
C	-0.7391242	2.4865630	3.7557042
C	0.6699538	2.0830578	3.2688769
O	1.6507814	2.7639130	4.0562242
H	0.8271147	0.9772461	3.3637281
H	-0.6382227	3.4994286	4.1887893
H	-1.1418157	1.8179447	4.5412082
H	-2.7872659	4.1939435	3.4470424
H	-3.6467351	3.4134939	2.0851011
H	-1.6194588	0.3658960	2.2251528
H	-2.8420790	1.2231488	1.2313049
H	-3.1084730	1.0130681	2.9972945
H	2.4373188	2.9079771	3.4943866
H	1.2225397	4.1844221	-0.3036934
H	3.3950217	4.4673320	-1.4750040
H	5.3977668	3.1140127	-0.7826433
H	5.1788400	1.4575048	1.0936389
H	2.9992346	1.1467536	2.2441117
H	-0.2771246	2.3030667	-1.4245455
H	-1.7167554	3.3629892	-3.1863523
H	-3.4786852	5.0213318	-2.5494442
H	-3.8139292	5.6562865	-0.1480344
Pd	-1.5893347	5.5928729	2.0620372
P	-0.4837331	6.7257824	3.7340213
C	-0.8337755	8.4864392	4.1440185
C	-1.1055613	9.3630666	3.0730291
H	-1.1393217	8.9635036	2.0463315
C	-1.3389032	10.7249479	3.3146496
H	-1.5488639	11.4026299	2.4732047
C	-1.3174026	11.2194799	4.6304262
H	-1.5091036	12.2863383	4.8213921
C	-1.0606475	10.3482716	5.7022695
H	-1.0497150	10.7315958	6.7341493
C	-0.8175411	8.9859876	5.4625963
H	-0.6219117	8.3025727	6.3027433
C	1.3494425	6.6841785	3.5660498
C	1.8968780	5.7258990	2.6904176
H	1.2120697	5.0881624	2.1105146
C	3.2886715	5.5921309	2.5667190
H	3.7053058	4.8453687	1.8746655

C	4.1388770	6.4211863	3.3171234
H	5.2307092	6.3204609	3.2196258
C	3.5973453	7.3878150	4.1833750
H	4.2638288	8.0442328	4.7636076
C	2.2059525	7.5214043	4.3093238
H	1.7833447	8.2800033	4.9853604
C	-0.7685374	5.8566331	5.3327968
C	0.2481572	5.1424378	5.9952221
H	1.2700305	5.1392326	5.5936134
C	-0.0566646	4.3853379	7.1390050
H	0.7418163	3.8146873	7.6364264
C	-1.3692758	4.3421343	7.6326367
H	-1.6045726	3.7452338	8.5268542
C	-2.3882050	5.0546769	6.9729470
H	-3.4212170	5.0200569	7.3515579
C	-2.0926620	5.7996356	5.8237379
H	-2.8933766	6.3392077	5.2928240

S4

73

SCF Energy = -1973.505801767

C	0.2975208	3.6848534	-1.8461033
C	0.0277904	3.4116733	-0.4860497
C	-1.3315031	3.3688601	-0.0531736
C	-2.3756205	3.3582004	-1.0098844
C	-2.0800201	3.6011370	-2.3667121
C	-0.7493931	3.8045429	-2.7718781
C	1.0099090	3.0162505	0.5236112
C	2.2507923	2.4420933	0.4470348
C	3.0846492	2.1104152	-0.7248690
C	4.4776585	2.3623346	-0.6977233
C	5.2909739	2.0073896	-1.7842784
C	4.7350865	1.3808220	-2.9117290
C	3.3579163	1.0979920	-2.9378163
C	2.5418476	1.4551516	-1.8561150
C	0.4656541	3.0228908	1.9548555
C	0.5915007	4.4201757	2.6042649
C	-0.9977186	2.5912381	1.8571911
C	1.4150816	2.0157718	2.6588217
C	2.7357255	2.0845018	1.8524047
O	3.6996631	3.0272295	2.3507325
H	3.2732391	1.1138719	1.8634068
H	1.5758677	2.2326884	3.7333144
H	1.0030378	0.9892463	2.5717190
H	-1.1152858	1.5704984	1.4505144
H	-1.5456139	2.6528986	2.8239593

H	1.6545608	4.7049202	2.7387661
H	0.1154611	4.4340158	3.6049847
H	0.0918712	5.1950105	1.9865285
H	3.3561746	3.9138203	2.1258413
H	4.9081594	2.8381685	0.1957344
H	6.3706124	2.2197950	-1.7477213
H	5.3740236	1.1024086	-3.7636018
H	2.9164309	0.5852576	-3.8063027
H	1.4693245	1.2131338	-1.8731692
H	-3.4198978	3.1862167	-0.7036103
H	-2.8970561	3.6368006	-3.1040851
H	-0.5213400	4.0200338	-3.8267076
H	1.3399636	3.7791674	-2.1803055
Pd	-2.2726728	4.3609784	1.4503031
P	-3.2729623	5.7816147	2.9288097
C	-2.0527432	6.3720301	4.1733435
C	-2.0035624	5.8349952	5.4752251
H	-2.7835633	5.1338232	5.8072435
C	-0.9591582	6.1885424	6.3461492
H	-0.9285495	5.7613241	7.3601300
C	0.0392993	7.0830023	5.9287753
H	0.8564943	7.3579684	6.6124628
C	-0.0082438	7.6245315	4.6314070
H	0.7720558	8.3248261	4.2964963
C	-1.0418204	7.2662093	3.7558425
H	-1.0639505	7.6756740	2.7337809
C	-4.6330941	5.0939020	3.9702802
C	-5.4526892	5.9037290	4.7831798
H	-5.3158112	6.9953029	4.7885842
C	-6.4491657	5.3203665	5.5795974
H	-7.0877725	5.9577143	6.2101254
C	-6.6351752	3.9262862	5.5707234
H	-7.4191896	3.4721768	6.1957479
C	-5.8254991	3.1159944	4.7584383
H	-5.9727723	2.0253982	4.7429039
C	-4.8299790	3.6986575	3.9570868
H	-4.1927114	3.0829595	3.3008672
C	-3.9954201	7.3426526	2.2662399
C	-4.0290296	8.5498015	2.9954942
H	-3.5712576	8.5991872	3.9951357
C	-4.6252121	9.6926798	2.4392363
H	-4.6440381	10.6325048	3.0120086
C	-5.1922119	9.6394441	1.1545777
H	-5.6562839	10.5378174	0.7199336
C	-5.1544523	8.4415010	0.4208332
H	-5.5859295	8.3991018	-0.5907146

C	-4.5526175	7.2998863	0.9713406
H	-4.4967624	6.3616913	0.3952797

Optimized Geometries (BXnf')

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R3
73
SCF Energy = -1973.572264771
C      2.2534145   -1.4973505   -1.3856451
C      0.9945981   -2.1678731   -1.1445793
C      0.1034437   -2.3823948   -2.2177615
C      0.3863066   -1.8260701   -3.4792723
C      1.5531135   -1.0675788   -3.6932481
C      2.5345645   -0.9355463   -2.6624457
C      0.9985236   -2.6070575    0.2464854
C      0.3410814   -3.5185585    1.0346495
C     -0.9480008   -4.1863641    0.8253433
C     -1.9870373   -3.5753952    0.0785532
C     -3.2264747   -4.2035398   -0.0989712
C     -3.4681060   -5.4644051    0.4728073
C     -2.4588856   -6.0785410    1.2339850
C     -1.2217186   -5.4465456    1.4144786
C      2.2479430   -2.0356133    0.9504073
C      1.9765137   -0.6900957    1.6589956
C      3.2120253   -1.7685558   -0.2337211
C      2.5350687   -3.1371944    1.9884713
C      1.1300449   -3.7108048    2.3335977
O      0.4757193   -3.0980070    3.4483856
H      1.2141755   -4.7815894    2.6149855
H      3.1404224   -3.9448264    1.5256472
H      3.0584844   -2.7853325    2.8991456
H      3.7981183   -2.6825955   -0.4794123
H      3.9306856   -0.9465882   -0.0497842
H      1.1609255   -0.7618325    2.4017094
H      1.7081743    0.0890764    0.9174296
H      2.8924435   -0.3643530    2.1928887
H      0.0972809   -2.2538236    3.1297903
H     -1.8206445   -2.5748780   -0.3408740
H     -4.0141015   -3.6986764   -0.6791070
H     -4.4408737   -5.9601679    0.3356732
H     -2.6391038   -7.0613857    1.6957440
H     -0.4469919   -5.9407343    2.0176647
H     -0.8145588   -2.9651243   -2.0735987

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H	-0.3261157	-1.9659948	-4.3056117
H	1.7510378	-0.6301187	-4.6828941
H	3.5348669	-0.5371466	-2.8952248
Pd	1.3909952	0.6162356	-1.5695581
P	0.0312302	2.0353334	-0.4820210
C	-1.4858650	2.6088351	-1.3569344
C	-1.3929966	2.8467249	-2.7439086
H	-0.4378790	2.6475297	-3.2567290
C	-2.5072579	3.3121650	-3.4575652
H	-2.4268725	3.4958491	-4.5398172
C	-3.7276704	3.5290527	-2.7941639
H	-4.6048634	3.8845179	-3.3559911
C	-3.8293666	3.2808419	-1.4150780
H	-4.7857593	3.4420309	-0.8943869
C	-2.7128296	2.8240813	-0.6958642
H	-2.7946193	2.6238562	0.3832017
C	0.7646443	3.5957616	0.1694097
C	2.1400705	3.5793253	0.4831450
H	2.7182441	2.6620616	0.2821032
C	2.7545245	4.7156011	1.0303578
H	3.8273192	4.6941664	1.2754371
C	2.0031819	5.8829684	1.2515286
H	2.4863953	6.7782299	1.6716816
C	0.6364439	5.9089587	0.9259919
H	0.0478789	6.8245792	1.0901672
C	0.0159813	4.7692960	0.3891862
H	-1.0543503	4.7924653	0.1351230
C	-0.6634228	1.2511215	1.0425442
C	-0.4698680	1.7834272	2.3321563
H	0.0407775	2.7494822	2.4551115
C	-0.9068807	1.0714807	3.4626062
H	-0.7380658	1.4886111	4.4670513
C	-1.5556382	-0.1652381	3.3143583
H	-1.8976871	-0.7213801	4.2003401
C	-1.7629184	-0.6953524	2.0263031
H	-2.2633307	-1.6671733	1.9019289
C	-1.3084323	0.0038645	0.8999293
H	-1.4237357	-0.4273596	-0.1074725

R4

73

SCF Energy = -1973.572492206

C	1.8513723	-4.3126501	2.1127389
C	0.9567141	-4.1464560	1.0245913
C	1.3053208	-4.7327426	-0.2162790
C	2.5219701	-5.4092436	-0.3801635

C	3.4181140	-5.5267403	0.6965691
C	3.0701912	-4.9833145	1.9454543
C	-0.2877896	-3.3932067	1.2085274
Pd	-1.4718943	0.7526084	-1.7126496
P	-0.0878019	2.1516857	-0.6251619
C	-0.9597383	-2.5690903	0.3465944
C	-0.9332276	-2.1349336	-1.0431215
C	0.0402741	-2.2428407	-2.0594288
C	-0.2015006	-1.6562559	-3.3133531
C	-1.4231560	-1.0012488	-3.5882443
C	-2.4714206	-0.9677092	-2.6143373
C	-2.1947838	-1.4964042	-1.3202458
C	-1.0536654	-3.4437300	2.5415708
O	-1.0075452	-4.6970765	3.2011196
C	-2.4751761	-2.9666492	2.1375907
C	-2.1844951	-1.9367193	1.0302721
C	-3.1551926	-1.7084011	-0.1556387
C	-1.8276644	-0.5702833	1.6573097
H	-0.6102945	-2.7262373	3.2707083
H	-3.0560184	-2.5700961	2.9940357
H	-3.0188620	-3.8412443	1.7179991
H	-3.7591417	-2.6235476	-0.3502239
H	-3.8577559	-0.8660481	-0.0048858
H	-2.6992002	-0.1639087	2.2100740
H	-1.5552168	0.1491690	0.8597354
H	-0.9689445	-0.6411057	2.3515202
H	-1.1886915	-5.3775068	2.5237692
H	0.5938280	-4.6751628	-1.0516235
H	2.7689663	-5.8573665	-1.3549760
H	4.3754638	-6.0537891	0.5674272
H	3.7555094	-5.0869294	2.8007178
H	1.5823537	-3.9051242	3.0965921
H	-3.4902081	-0.6552995	-2.8952436
H	-1.6058309	-0.5866633	-4.5907131
H	0.5730708	-1.6961857	-4.0933341
H	1.0002648	-2.7366947	-1.8607798
C	1.1812878	3.0675970	-1.5982148
C	0.9301100	1.1608526	0.5575267
C	-0.8041789	3.4685913	0.4483322
C	-0.0868829	4.6206541	0.8297412
C	-0.6759780	5.5655464	1.6849616
C	-1.9812209	5.3662042	2.1665056
C	-2.7024515	4.2222235	1.7837790
C	-2.1191266	3.2809642	0.9221014
H	0.9343407	4.7795122	0.4517204
H	-0.1123090	6.4652156	1.9759501

H	-2.4407230	6.1093449	2.8359460
H	-3.7284844	4.0673526	2.1508400
H	-2.6771754	2.3879386	0.5966920
C	2.5167903	3.2073156	-1.1690370
C	3.4337784	3.9340666	-1.9465914
C	3.0235627	4.5285210	-3.1512498
C	1.6929432	4.3887027	-3.5841997
C	0.7778911	3.6547639	-2.8157275
H	2.8386302	2.7385389	-0.2267973
H	4.4764580	4.0351980	-1.6082741
H	3.7443597	5.0960544	-3.7593793
H	1.3700351	4.8454591	-4.5321992
H	-0.2610105	3.5193858	-3.1577285
C	1.0235229	1.4486069	1.9322895
C	1.6856296	0.5550820	2.7937854
C	2.2599285	-0.6222264	2.2889958
C	2.1875766	-0.9016340	0.9120250
C	1.5258355	-0.0159634	0.0535172
H	0.5559875	2.3582368	2.3366325
H	1.7412061	0.7789158	3.8702533
H	2.7604369	-1.3314777	2.9650818
H	2.6270538	-1.8289092	0.5156727
H	1.4279094	-0.2512518	-1.0171428

S3

73

SCF Energy = -1973.578348420

C	-2.9217349	-1.3809345	0.9514153
C	-1.9116775	-1.9853870	0.1150032
C	-2.1764439	-2.1742892	-1.2826319
C	-3.4203817	-1.7118396	-1.8031075
C	-4.3919993	-1.1368270	-0.9664575
C	-4.1500679	-0.9865243	0.4185290
C	-0.8138476	-2.4297269	0.9884495
C	0.5063485	-2.7798895	0.9432279
C	1.4358374	-2.9815424	-0.1760848
C	1.3243492	-2.2757745	-1.3971186
C	2.2957638	-2.3935964	-2.3959170
C	3.4087675	-3.2319051	-2.2118819
C	3.5326735	-3.9563763	-1.0154642
C	2.5618470	-3.8318366	-0.0099813
C	-1.3276873	-2.3745743	2.4345291
C	-1.9699456	-3.7317453	2.8057247
C	-2.4274618	-1.2849972	2.3816712
C	-0.0278529	-2.1319242	3.2205892
C	1.0468573	-2.8581691	2.3866710

O	2.2980764	-2.1978679	2.5597188
H	1.1392108	-3.9268566	2.7125582
H	0.2284768	-1.0521399	3.2066960
H	-0.0617357	-2.4709678	4.2748776
H	-1.9812094	-0.2814064	2.5543694
H	-3.2338205	-1.4263631	3.1293625
H	-1.2408046	-4.5617925	2.7195013
H	-2.8229990	-3.9600055	2.1348362
H	-2.3488917	-3.7071913	3.8483749
H	2.9069416	-2.5722324	1.8911637
H	0.4847228	-1.5599810	-1.5311571
H	2.1930213	-1.8025966	-3.3184741
H	4.1769557	-3.3178305	-2.9950682
H	4.3919229	-4.6272576	-0.8621343
H	2.6638468	-4.4320042	0.9087550
H	-1.5171313	-2.7996754	-1.9026117
H	-3.6361129	-1.8584651	-2.8719222
H	-5.3508880	-0.8092250	-1.3944546
H	-4.9203635	-0.5472670	1.0708052
Pd	-1.1772563	-0.2060739	-1.1061985
P	0.1842702	1.4979662	-0.6078171
C	0.1229852	3.0700046	-1.5727439
C	-0.5730164	3.0673289	-2.7970814
H	-1.0798541	2.1408787	-3.1152638
C	-0.6208482	4.2281148	-3.5868479
H	-1.1652873	4.2189591	-4.5434161
C	0.0187106	5.3996531	-3.1501614
H	-0.0229577	6.3120832	-3.7645077
C	0.7075503	5.4093015	-1.9236925
H	1.2045982	6.3286525	-1.5780193
C	0.7617164	4.2492409	-1.1373355
H	1.2985812	4.2597908	-0.1766259
C	1.9577801	1.0200866	-0.7263888
C	2.5105625	0.1417362	0.2313994
H	1.9266188	-0.1959568	1.1004330
C	3.8194319	-0.3339284	0.0750515
H	4.2418479	-1.0087347	0.8336439
C	4.5799741	0.0283962	-1.0480475
H	5.6001792	-0.3637623	-1.1748008
C	4.0282628	0.8883222	-2.0115374
H	4.6161727	1.1772851	-2.8962336
C	2.7269317	1.3894750	-1.8492650
H	2.3025312	2.0688915	-2.6035943
C	-0.0199302	2.0726869	1.1336259
C	1.0499572	2.4711191	1.9603820
H	2.0812103	2.4360049	1.5792410

C	0.8039715	2.8912276	3.2781214
H	1.6464702	3.1884746	3.9210796
C	-0.5089942	2.9295046	3.7756881
H	-0.6974996	3.2560138	4.8097131
C	-1.5804173	2.5420053	2.9519501
H	-2.6109667	2.5649501	3.3379585
C	-1.3363067	2.1068343	1.6410423
H	-2.1626633	1.7670893	0.9946782

S4

73

SCF Energy = -1973.576018477

C	2.2251782	0.1760437	-2.0551306
C	2.1557383	-0.8726729	-1.1129428
C	1.5537616	-2.1282933	-1.4725831
C	0.9918305	-2.3184907	-2.7673209
C	0.9824680	-1.2008515	-3.6619902
C	1.6208657	0.0119758	-3.3127112
C	2.5911961	-0.9824926	0.2736407
C	3.4529068	-0.3696737	1.1427069
C	4.2391179	0.8605442	0.9829640
C	4.4541510	1.7083472	2.0998856
C	5.1846903	2.8976185	1.9675059
C	5.7318927	3.2619784	0.7254421
C	5.5567905	2.4128658	-0.3815616
C	4.8226640	1.2256723	-0.2543242
C	1.9704987	-2.2555404	0.8790527
C	0.5637976	-2.0134278	1.4678099
C	1.8098365	-3.1564971	-0.3769057
C	2.9737288	-2.5741012	2.0054326
C	3.4971058	-1.1748163	2.4447742
O	2.7479460	-0.5564390	3.5039651
H	4.5320559	-1.2423293	2.8414230
H	2.5419563	-3.1296722	2.8611251
H	3.8283712	-3.1573085	1.6028151
H	2.7613788	-3.6890754	-0.6005581
H	1.0084026	-3.9151485	-0.2863992
H	0.5622195	-1.2296765	2.2461903
H	0.1854355	-2.9492186	1.9269977
H	-0.1411062	-1.7059842	0.6692120
H	1.9469704	-0.1636593	3.0999376
H	4.0198349	1.4182574	3.0680625
H	5.3289494	3.5472349	2.8446336
H	6.3038340	4.1965700	0.6226025
H	6.0066792	2.6731195	-1.3521731
H	4.7218267	0.5492537	-1.1145584

H	0.6887842	-3.3194238	-3.1145109
H	0.5523901	-1.3193412	-4.6675633
H	1.6299673	0.8404582	-4.0362147
H	2.7013896	1.1300482	-1.7930744
Pd	-0.7407652	-1.3835852	-1.7999288
P	-2.1227373	-0.0740647	-0.6068290
C	-1.1300304	0.8134178	0.6785051
C	-1.4146480	0.7569692	2.0558657
H	-2.3234183	0.2480193	2.4087870
C	-0.5209535	1.3237357	2.9834553
H	-0.7439452	1.2641279	4.0597908
C	0.6557527	1.9520232	2.5421319
H	1.3593730	2.3876842	3.2672986
C	0.9323255	2.0285062	1.1634929
H	1.8582355	2.5096659	0.8154444
C	0.0460807	1.4613395	0.2406337
H	0.2794981	1.4816055	-0.8345808
C	-3.4695514	-0.8506261	0.3843977
C	-4.6125073	-0.1450927	0.8121932
H	-4.7471960	0.9075618	0.5211209
C	-5.5798843	-0.7856935	1.6027622
H	-6.4725170	-0.2308222	1.9300069
C	-5.4118529	-2.1308109	1.9738988
H	-6.1723925	-2.6302807	2.5932571
C	-4.2768535	-2.8399112	1.5446596
H	-4.1462528	-3.8961414	1.8251905
C	-3.3133964	-2.2047329	0.7464695
H	-2.4271707	-2.7514836	0.3851530
C	-2.9880705	1.3029373	-1.4729350
C	-3.1346503	2.5868583	-0.9090992
H	-2.7015208	2.8015857	0.0795171
C	-3.8219772	3.5901941	-1.6119562
H	-3.9285664	4.5920347	-1.1683777
C	-4.3701136	3.3178415	-2.8762576
H	-4.9066519	4.1062605	-3.4257674
C	-4.2232137	2.0395608	-3.4433266
H	-4.6431990	1.8253780	-4.4379544
C	-3.5283327	1.0387555	-2.7487936
H	-3.3857014	0.0407587	-3.1940408

Optimized Geometries (TS-BXne'-f')

R3

79

SCF Energy = -2238.392395776

C	0.1332109	8.5162110	0.9223545
C	-0.7971417	7.5657802	1.4008893
C	-0.7881010	7.2213357	2.7667477
C	0.1416588	7.8126538	3.6386052
C	1.0596419	8.7595495	3.1588309
C	1.0484672	9.1159701	1.7977899
P	-1.8544049	6.7211059	0.1488755
C	-2.8122644	5.5281623	1.1749685
C	-3.9268072	5.9003825	1.9507288
C	-4.5839720	4.9407606	2.7384992
C	-4.1329139	3.6097454	2.7566775
C	-3.0273033	3.2294496	1.9764965
C	-2.3734045	4.1881483	1.1855605
Pd	-0.5314630	5.6627788	-1.4296271
C	1.6603321	5.6456312	-1.1096694
C	2.0423786	4.5536171	-0.0904761
C	1.1891330	3.3190202	-0.4121248
C	0.7276655	2.6870885	0.7059618
C	1.2182603	3.4485233	1.9532002
C	1.6459243	4.8221584	1.3761571
C	-0.2072231	1.5567826	0.7895639
C	-0.3422131	0.8116335	1.9878491
C	-1.2840608	-0.2238510	2.0915926
C	-2.1241711	-0.5381386	1.0107769
C	-2.0045727	0.1947062	-0.1851171
C	-1.0619707	1.2246434	-0.2944638
C	0.9996060	3.2046419	-1.8610563
C	1.1272918	2.0600638	-2.6708275
C	1.0266603	2.1797515	-4.0667210
C	0.8123457	3.4438339	-4.6570945
C	0.7084817	4.6011513	-3.8585563
C	0.7748183	4.4891829	-2.4492427
O	0.2754850	3.5449777	3.0108164
C	3.5397761	4.2006290	-0.2255616
O	-2.0008424	2.8653848	-3.0724517
C	-3.1060591	7.9978223	-0.2813358
C	-3.3248806	9.1520504	0.4983699
C	-4.3169553	10.0734619	0.1246633
C	-5.0951243	9.8449676	-1.0225218
C	-4.8753695	8.6955250	-1.8019644
C	-3.8799317	7.7748855	-1.4411492
H	2.0881986	2.9215830	2.4082813
H	2.4341792	5.3212967	1.9727005
H	0.7499840	5.4744969	1.3918993

H	1.3929949	6.6071794	-0.6148157
H	2.4595365	5.8772001	-1.8367576
H	4.1676620	5.0911009	-0.0162463
H	3.7676916	3.8486394	-1.2525378
H	3.8306649	3.3973954	0.4813139
H	-0.5584345	3.8925809	2.6303358
H	-0.9939190	1.7932914	-1.2306065
H	-2.6485221	-0.0457133	-1.0465725
H	-2.8652303	-1.3469475	1.0972804
H	-1.3678104	-0.7861800	3.0342499
H	0.2753286	1.0741730	2.8564134
H	-1.2895349	3.2281461	-3.6588516
H	0.5469946	5.5819232	-4.3312325
H	0.7389975	3.5312421	-5.7524507
H	1.1239463	1.2874003	-4.7027621
H	1.3059663	1.0795690	-2.2051073
H	-4.2843857	6.9411347	1.9319597
H	-5.4570016	5.2349141	3.3410294
H	-4.6513034	2.8607948	3.3744058
H	-2.6757272	2.1878320	1.9763455
H	-1.5248916	3.9070599	0.5396914
H	-2.7141967	9.3304191	1.3963696
H	-4.4828293	10.9749773	0.7343240
H	-5.8717110	10.5687644	-1.3136728
H	-5.4785948	8.5181258	-2.7054290
H	-3.6890931	6.8794231	-2.0544892
H	-1.4978207	6.4739295	3.1492091
H	0.1497910	7.5231059	4.7002478
H	1.7895207	9.2178282	3.8431554
H	1.7659928	9.8576446	1.4148854
H	0.1371543	8.7772282	-0.1484170
C	-2.7202244	3.8969285	-2.5871301
O	-2.6532568	5.0513136	-2.9775930
O	-3.5587102	3.5062538	-1.6160809
H	-3.3250642	2.5968965	-1.3291701

R4

79

SCF Energy = -2238.381672208

C	-2.3711864	6.3405158	5.3366655
C	-0.9661016	6.2766146	5.2039513
C	-0.2159350	5.5447594	6.1451606
C	-0.8648237	4.8798829	7.1997522
C	-2.2611076	4.9472240	7.3278283
C	-3.0132518	5.6868437	6.3967874
P	-0.2153530	7.0478032	3.7057655

C	1.5715503	6.6674737	3.9118234
C	2.0338620	5.4788968	3.3101676
C	3.3663484	5.0733461	3.4719798
C	4.2491579	5.8679667	4.2235591
C	3.7980308	7.0639677	4.8094164
C	2.4605928	7.4655818	4.6584973
Pd	-1.1027346	6.0445600	1.8221389
O	1.0025337	6.6800467	0.2383826
C	0.5542707	7.6089806	-0.4070122
O	-0.6003958	8.2604914	-0.1479972
C	-1.7881780	4.9390522	0.2491820
C	-0.9635656	3.7904152	0.0759210
C	-0.6016719	3.3726491	-1.2176400
C	-1.1029921	4.0666382	-2.3320192
C	-1.9747587	5.1591335	-2.1611225
C	-2.3338303	5.5952008	-0.8713411
C	-0.6929634	3.1359157	1.3592020
C	0.4003949	2.6029885	1.9743090
C	0.0217578	2.1802465	3.3894838
C	-1.2875971	2.9621910	3.6553051
C	-1.9366939	3.1527276	2.2638646
C	1.7814465	2.5154596	1.4821367
C	2.6581442	1.5346257	2.0076064
C	4.0020873	1.4869054	1.6080094
C	4.4991912	2.4189979	0.6809793
C	3.6385959	3.4019438	0.1584722
C	2.2955581	3.4530453	0.5511715
C	-2.8544960	1.9655470	1.8978610
C	-2.6732778	4.4908477	2.0380272
O	-0.1352902	0.7485200	3.4157061
C	-0.3249506	8.8466698	4.0819708
C	-0.2136364	9.7621933	3.0147225
C	-0.2439033	11.1429045	3.2616978
C	-0.3963915	11.6219710	4.5740489
C	-0.5178265	10.7145861	5.6396607
C	-0.4806847	9.3320666	5.3972827
O	1.1836057	8.1214039	-1.4798645
H	0.6187782	8.8297437	-1.8509834
H	0.8218110	2.4794429	4.1088346
H	-1.0267588	3.9532118	4.0749474
H	-1.9450249	2.4504217	4.3877501
H	-2.8746526	5.0329173	2.9874589
H	-3.6355307	4.3880778	1.5078083
H	-2.3238606	1.0107898	2.0800943
H	-3.1504419	2.0130757	0.8299115
H	-3.7764065	1.9850826	2.5158956

H	-0.2851494	0.4988272	4.3469086
H	2.2556736	0.7994342	2.7200321
H	4.6673383	0.7142714	2.0237913
H	5.5551994	2.3851397	0.3722041
H	4.0213999	4.1546819	-0.5473406
H	1.6541329	4.2633886	0.1772349
H	0.0548169	2.4993980	-1.3462424
H	-0.8316239	3.7375812	-3.3464509
H	-2.3835191	5.6764403	-3.0433405
H	-3.0147870	6.4510331	-0.7469121
H	-1.0591259	7.7228247	0.5880232
H	-0.1135000	9.3897654	1.9844650
H	-0.1564183	11.8493462	2.4222793
H	-0.4268053	12.7052773	4.7660774
H	-0.6421265	11.0850001	6.6687631
H	-0.5766663	8.6225222	6.2327762
H	1.3393041	4.8795341	2.7022915
H	3.7121452	4.1451478	2.9937899
H	5.2987591	5.5589073	4.3441268
H	4.4935596	7.6913108	5.3879205
H	2.1080133	8.4009772	5.1186106
H	0.8774309	5.4850770	6.0436794
H	-0.2712477	4.3040874	7.9263137
H	-2.7666804	4.4219433	8.1522010
H	-4.1082487	5.7443052	6.4921329
H	-2.9591509	6.9039872	4.5943436

S3

79

SCF Energy = -2238.392793926

C	-2.6741508	5.8949928	6.1749519
C	-1.3435203	6.3498857	6.0698608
C	-0.6322267	6.7011208	7.2356412
C	-1.2514371	6.6015803	8.4917664
C	-2.5808926	6.1568608	8.5911227
C	-3.2924542	5.8051680	7.4310938
P	-0.6107765	6.4869541	4.3894552
C	1.1968115	6.3771362	4.7038829
C	1.6930488	5.1643555	5.2287258
C	3.0695163	4.9820756	5.4032146
C	3.9659560	6.0014499	5.0364981
C	3.4771346	7.2065009	4.5093915
C	2.0943766	7.4007934	4.3481400
Pd	-1.4327560	4.9322009	2.8853269
C	-1.7699947	2.7831271	2.9076262
C	-0.6718868	1.9286326	2.2601062

C	-0.1785525	2.6087095	0.9733239
C	1.1572158	2.4163798	0.7725368
C	1.7364401	1.6219529	1.9645068
C	0.6455741	1.8035932	3.0494864
C	-1.2637269	3.3421876	0.3160204
C	-2.1500113	3.9737751	1.2354419
C	-3.3489103	4.5618213	0.7842969
C	-3.6279319	4.5920963	-0.5954763
C	-2.7340563	4.0084428	-1.5113761
C	-1.5621274	3.3793404	-1.0617671
C	2.0212380	2.9024770	-0.3128880
C	1.6808453	4.0336843	-1.0964842
C	2.5413147	4.5075641	-2.0943603
C	3.7626611	3.8593771	-2.3475549
C	4.1181692	2.7396239	-1.5771019
C	3.2661634	2.2718283	-0.5669610
C	-1.2573190	0.5411138	1.9044572
O	3.0269492	2.0084686	2.3778248
O	2.5321587	4.6988487	2.2917855
C	-0.8807024	8.2501449	3.9322142
C	-0.6760360	8.6248612	2.5855214
C	-0.8526992	9.9602727	2.1937022
C	-1.2509736	10.9264891	3.1335131
C	-1.4654226	10.5541599	4.4706911
C	-1.2780698	9.2217666	4.8726468
H	1.8236089	0.5448644	1.6857699
H	0.8572107	2.7698212	3.5544170
H	0.6437784	0.9951881	3.8077612
H	-1.5849259	2.9699733	3.9915316
H	-2.7851990	2.3626484	2.8034285
H	-0.4950453	-0.1092573	1.4310018
H	-2.1008438	0.6475016	1.1921798
H	-1.6331600	0.0296977	2.8149463
H	3.0045165	2.9929331	2.4336826
H	0.7472481	4.5723713	-0.8930212
H	2.2573416	5.3991580	-2.6739644
H	4.4369642	4.2305377	-3.1345142
H	5.0761224	2.2278657	-1.7581466
H	3.5757483	1.4240756	0.0573299
H	-0.8836369	2.8894827	-1.7755419
H	-2.9659705	4.0215733	-2.5871909
H	-4.5542734	5.0669625	-0.9538529
H	-4.0578869	5.0086228	1.4982561
H	0.2993838	5.4225124	1.8055314
H	-0.3616812	7.8701765	1.8488182
H	-0.6845276	10.2444876	1.1439715

H	-1.3988394	11.9716298	2.8217795
H	-1.7817430	11.3061321	5.2096411
H	-1.4469907	8.9353280	5.9209329
H	0.9927672	4.3532478	5.4818716
H	3.4475165	4.0273835	5.7979030
H	5.0493839	5.8501392	5.1566638
H	4.1742517	8.0079887	4.2207728
H	1.7149993	8.3456205	3.9327671
H	0.4096735	7.0462103	7.1567327
H	-0.6910338	6.8722961	9.3995860
H	-3.0621196	6.0771844	9.5777080
H	-4.3310651	5.4491662	7.5062641
H	-3.2128582	5.6028750	5.2582971
C	2.2005934	5.6275469	1.5679044
O	0.9576536	6.0063599	1.2883265
O	3.0717619	6.4374727	0.9366711
H	3.9569010	6.0769812	1.1478961

S4

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SCF Energy = -2238.386373030

C	-2.8212156	4.9405271	0.5537775
C	-3.0642795	4.9789334	1.9438789
C	-4.0794851	4.1696990	2.4905812
C	-4.8399921	3.3350860	1.6529703
C	-4.6066806	3.3173844	0.2679561
C	-3.5985473	4.1286714	-0.2814696
P	-1.9845502	6.0839201	2.9510388
C	-2.6637495	5.8674609	4.6546045
C	-3.6272506	6.7369602	5.2050433
C	-4.1242300	6.5131990	6.4994407
C	-3.6719690	5.4177869	7.2531996
C	-2.7115631	4.5469358	6.7102108
C	-2.2041209	4.7765883	5.4231195
Pd	0.2353310	5.5534891	2.5520114
C	1.1337703	3.7274071	3.4206324
C	0.6472617	2.4935036	2.6342610
C	0.6772372	2.8780702	1.1455762
C	-0.4003784	2.4084150	0.4538608
C	-1.3071713	1.6249716	1.4008427
C	-0.8353220	2.0896779	2.8037744
C	1.8056815	3.7699825	0.8688575
C	2.7233688	3.7064714	-0.1970549
C	3.8271739	4.5749930	-0.2169147
C	4.0200038	5.5001567	0.8324136
C	3.1154099	5.5631686	1.9119852

C	1.9798497	4.7196220	1.9248755
C	-0.7732429	2.6477077	-0.9454624
C	-1.6524846	1.7538949	-1.6040371
C	-2.0930945	2.0118069	-2.9102489
C	-1.6707321	3.1677781	-3.5884052
C	-0.7887575	4.0583522	-2.9471298
C	-0.3412840	3.8020782	-1.6448311
C	1.6044013	1.3089813	2.8953052
O	-1.2442111	0.2043109	1.1797430
O	0.6476968	7.7084354	1.1691062
C	-2.5900919	7.7610348	2.4952084
C	-1.7668188	8.8592210	2.8179426
C	-2.1882525	10.1645958	2.5271193
C	-3.4254336	10.3822085	1.8964295
C	-4.2431014	9.2897408	1.5621379
C	-3.8298482	7.9818219	1.8624375
H	-2.3729456	1.8843248	1.2387893
H	-1.0123464	1.3118347	3.5724503
H	-1.4229991	2.9909315	3.0694164
H	0.4545159	4.0172962	4.2530027
H	2.1328245	3.5944834	3.8738492
H	1.2801463	0.3984609	2.3523969
H	1.6295783	1.0636072	3.9770545
H	2.6359071	1.5549703	2.5695276
H	-0.3063501	-0.0071155	1.0097380
H	-1.9786207	0.8499727	-1.0688045
H	-2.7770731	1.3039979	-3.4034390
H	-2.0194881	3.3717708	-4.6120407
H	-0.4418684	4.9613021	-3.4755757
H	0.3324031	4.5141240	-1.1492985
H	2.2078371	6.4696415	-0.1402433
H	3.2752785	6.2917559	2.7209461
H	4.8911422	6.1737612	0.8142582
H	4.5476235	4.5297775	-1.0470773
H	2.5717298	2.9745296	-1.0042216
H	-0.7865289	8.6798971	3.2838186
H	-1.5398698	11.0170426	2.7805622
H	-3.7502803	11.4067171	1.6585311
H	-5.2108151	9.4559015	1.0643630
H	-4.4710952	7.1264820	1.6025779
H	-3.9887977	7.5930568	4.6168593
H	-4.8734832	7.2009028	6.9206913
H	-4.0647455	5.2441392	8.2665599
H	-2.3488608	3.6880942	7.2952192
H	-1.4457108	4.0988401	5.0034350
H	-4.2752872	4.1897232	3.5725546

H	-5.6238058	2.6968181	2.0887219
H	-5.2017200	2.6614917	-0.3849975
H	-3.3969351	4.1085780	-1.3622572
H	-2.0169176	5.5587547	0.1293865
C	0.4925570	7.2941333	0.0347835
O	-0.6678016	7.4240429	-0.6370801
O	1.4195492	6.6617514	-0.7110900
H	-0.5858858	6.9555428	-1.4940041

Optimized Geometries (BXnf“)

R3
79
SCF Energy = -2238.439527857

C	2.1137780	2.4886544	0.5899693
C	0.9536382	1.9716986	1.2090855
C	0.9712460	1.7181401	2.5963353
C	2.1346241	1.9697323	3.3471836
C	3.2815596	2.4879008	2.7261680
C	3.2642513	2.7536212	1.3451326
P	-0.4777610	1.5280615	0.1331710
C	-1.8537931	1.3079331	1.3400909
C	-2.7609191	2.3298472	1.6812351
C	-3.8120742	2.0635640	2.5743505
C	-3.9624867	0.7839918	3.1366623
C	-3.0558228	-0.2381484	2.8021774
C	-2.0114079	0.0228027	1.9021043
Pd	0.1014303	-0.2660091	-1.0752212
C	2.9326072	-0.7479858	-1.7249100
C	3.1567067	-1.6603565	-0.4829154
C	1.7714590	-2.2539501	-0.1923615
C	1.5757870	-2.4758055	1.1464198
C	2.7938024	-1.9256715	1.9175337
C	3.5111347	-1.0296535	0.8738328
C	0.4165100	-3.0389830	1.8443443
C	0.5345528	-3.5257575	3.1724520
C	-0.5718723	-4.0632986	3.8444771
C	-1.8312790	-4.1185984	3.2222900
C	-1.9723990	-3.6158485	1.9166878
C	-0.8664180	-3.0842091	1.2421319
C	1.0325787	-2.2872336	-1.4661865
C	0.0214556	-3.1469384	-1.9841683
C	-0.4074978	-2.9873068	-3.3113680

C	0.1222858	-1.9594063	-4.1254132
C	1.1370332	-1.1182445	-3.6452437
C	1.6425425	-1.2973694	-2.3327295
O	2.4680145	-1.2436194	3.1169872
C	4.1302348	-2.8021985	-0.8532982
O	-2.7003510	-1.6497887	-1.3704986
C	-0.8867756	3.1087555	-0.7083267
C	-0.5887213	4.3663623	-0.1416529
C	-0.9577458	5.5433231	-0.8116488
C	-1.6305983	5.4705547	-2.0436516
C	-1.9299544	4.2186134	-2.6071018
C	-1.5552587	3.0368287	-1.9487193
H	3.4561334	-2.7601634	2.2444265
H	4.5976229	-0.9274493	1.0657283
H	3.0537712	-0.0207983	0.9366648
H	2.8183771	0.3155248	-1.4297693
H	3.7725564	-0.8027460	-2.4492540
H	5.1395697	-2.3962746	-1.0716817
H	3.7758169	-3.3464225	-1.7527835
H	4.2218149	-3.5378593	-0.0294028
H	1.9189740	-0.4706936	2.8673489
H	-1.0105560	-2.6445368	0.2480979
H	-2.9533550	-3.6224278	1.4170154
H	-2.6967558	-4.5427189	3.7538716
H	-0.4497331	-4.4400562	4.8716730
H	1.5019739	-3.4622412	3.6867279
H	-2.0368844	-2.0669534	-1.9758101
H	1.5747123	-0.3469899	-4.2967505
H	-0.2601565	-1.8230252	-5.1468481
H	-1.1630680	-3.6727405	-3.7251444
H	-0.3817910	-3.9549820	-1.3578973
H	-2.6573911	3.3285965	1.2326008
H	-4.5251688	2.8628742	2.8276266
H	-4.7913329	0.5818080	3.8319642
H	-3.1557173	-1.2472109	3.2299563
H	-1.3159367	-0.7819115	1.6191334
H	-0.0619741	4.4230556	0.8230504
H	-0.7193151	6.5225099	-0.3686919
H	-1.9186722	6.3946817	-2.5678396
H	-2.4550488	4.1567643	-3.5722277
H	-1.7850682	2.0554185	-2.3945118
H	0.0695295	1.3289733	3.0926993
H	2.1412423	1.7567823	4.4266475
H	4.1899024	2.6800807	3.3159776
H	4.1595273	3.1595600	0.8500930
H	2.1080978	2.6829586	-0.4941472

C	-2.9703912	-0.4157592	-1.8716561
O	-2.6753241	-0.0267660	-2.9822609
O	-3.6554089	0.3302666	-0.9869144
H	-3.6110614	-0.0974957	-0.1035187

R4

79

SCF Energy = -2238.436633861

C	-2.3581003	2.4898521	1.1662024
C	-0.9878477	2.1879870	1.3330428
C	-0.4743737	2.0087191	2.6323144
C	-1.3237104	2.1169893	3.7472744
C	-2.6848118	2.4140043	3.5757960
C	-3.1992280	2.6087859	2.2808575
P	0.0302072	1.9437633	-0.1897257
C	1.6489035	1.4169547	0.4980224
C	1.7684038	0.0702885	0.8996964
C	2.9399470	-0.3745609	1.5286663
C	4.0095785	0.5155837	1.7272611
C	3.9038873	1.8509602	1.3034483
C	2.7221868	2.3078565	0.6971609
Pd	-1.1073159	0.4973140	-1.4594858
O	2.0848955	-1.3176182	-2.3275180
C	2.1984876	-0.3973718	-3.1072069
O	1.3102072	0.5925831	-3.3232337
C	-2.3898608	-1.3270639	-1.1260558
C	-1.3971984	-2.3515415	-0.9095663
C	-0.7402256	-2.9381398	-2.0041265
C	-0.9976320	-2.4675630	-3.3058036
C	-1.9074609	-1.4222245	-3.5268178
C	-2.6421596	-0.8536828	-2.4458388
C	-1.3032775	-2.5520499	0.5355621
C	-0.3598649	-2.8687030	1.4750582
C	-0.9159388	-2.5246517	2.8589942
C	-2.1105257	-1.5835410	2.5512103
C	-2.6095207	-2.0576667	1.1723375
C	1.0100799	-3.3778807	1.3250119
C	1.6348482	-4.0454667	2.4098295
C	2.9623398	-4.4875305	2.3115763
C	3.6998866	-4.2688447	1.1345934
C	3.0944664	-3.5998548	0.0562843
C	1.7673126	-3.1638836	0.1484486
C	-3.5993967	-3.2373990	1.2999516
C	-3.1532230	-1.0116496	0.1602511
O	-1.2929812	-3.7390626	3.5346431
C	0.3540588	3.6569546	-0.7767594

C	0.8889094	3.8224557	-2.0728560
C	1.1858188	5.1071515	-2.5508638
C	0.9391003	6.2353240	-1.7485723
C	0.4011586	6.0738278	-0.4613296
C	0.1126145	4.7890172	0.0273914
O	3.2845527	-0.2519008	-3.9033808
H	3.1540209	0.5593547	-4.4347328
H	-0.1326157	-1.9979518	3.4553148
H	-1.7354983	-0.5421618	2.4747962
H	-2.8805470	-1.6105941	3.3499197
H	-2.9563255	0.0228380	0.5071707
H	-4.2492384	-1.0953319	0.0051550
H	-3.1800759	-4.0136372	1.9681113
H	-3.8028048	-3.6915212	0.3083847
H	-4.5637337	-2.8847149	1.7224599
H	-1.5418133	-3.4919224	4.4450349
H	1.0481024	-4.2367778	3.3198457
H	3.4251442	-5.0103587	3.1630372
H	4.7436287	-4.6112422	1.0624368
H	3.6570529	-3.3804531	-0.8631860
H	1.3567429	-2.5845887	-0.6860671
H	-0.0197080	-3.7507111	-1.8466726
H	-0.4636339	-2.9140177	-4.1570019
H	-2.0943224	-1.0602981	-4.5487253
H	-3.4825655	-0.1711696	-2.6500914
H	0.5252849	0.4844860	-2.6618540
H	1.0759602	2.9371295	-2.7003823
H	1.6052579	5.2301127	-3.5610694
H	1.1640339	7.2430704	-2.1296651
H	0.2061815	6.9541068	0.1701554
H	-0.3022092	4.6632019	1.0385730
H	0.9334521	-0.6241533	0.7193801
H	3.0217107	-1.4238312	1.8452222
H	4.9347046	0.1615518	2.2070778
H	4.7449050	2.5459501	1.4502844
H	2.6323778	3.3577986	0.3814030
H	0.5900264	1.7710940	2.7715964
H	-0.9150437	1.9646680	4.7578692
H	-3.3482333	2.4918860	4.4503581
H	-4.2653814	2.8423588	2.1391136
H	-2.7604098	2.6162254	0.1478260

S3

79

SCF Energy = -2238.442284859

C	-1.7996814	-0.3876832	4.3629912
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C	-0.4539588	-0.5414774	3.9687231
C	0.4486956	-1.2062305	4.8234444
C	0.0083272	-1.7049782	6.0605494
C	-1.3301994	-1.5404542	6.4530919
C	-2.2337849	-0.8795747	5.6024008
P	0.0512395	0.1854818	2.3526369
C	1.6424265	-0.6628819	1.9834237
C	1.6083585	-2.0536910	1.7453699
C	2.7710761	-2.7325095	1.3618748
C	3.9734964	-2.0254650	1.1838931
C	4.0080058	-0.6399247	1.4041425
C	2.8488931	0.0416842	1.8119124
Pd	-1.5008018	0.0260200	0.7432027
C	-2.4390807	-2.1173083	-1.2008961
C	-1.8487784	-2.2769722	-2.6268531
C	-1.3093436	-0.8774814	-2.9610708
C	-0.1788480	-0.9365063	-3.7287797
C	0.2592671	-2.4130340	-3.8711373
C	-0.6066499	-3.1606536	-2.8213062
C	-2.1040990	0.0917489	-2.2065954
C	-2.7036594	-0.6170713	-1.0994221
C	-3.5491016	0.0739812	-0.1893720
C	-3.7894152	1.4635626	-0.3911755
C	-3.2436400	2.1267984	-1.5003794
C	-2.4083890	1.4501334	-2.4108683
C	0.6515428	0.1298845	-4.3045156
C	0.6258094	1.4621665	-3.8241590
C	1.4469372	2.4515421	-4.3781308
C	2.3124344	2.1436759	-5.4408207
C	2.3596824	0.8258977	-5.9265510
C	1.5512337	-0.1692287	-5.3618925
C	-2.9746215	-2.6399695	-3.6203909
O	1.6468298	-2.6079523	-3.6763548
O	1.6446801	-1.1504360	-1.3083434
C	0.5647339	1.8947567	2.8081982
C	0.3157029	2.9353057	1.8910597
C	0.7273294	4.2450090	2.1835702
C	1.3782084	4.5240186	3.3966184
C	1.6179323	3.4903505	4.3191884
C	1.2137507	2.1789275	4.0275743
H	0.0465453	-2.7842235	-4.9005917
H	-0.0190167	-3.1825356	-1.8814576
H	-0.8326959	-4.2051993	-3.1147372
H	-1.7012748	-2.4366289	-0.4337352
H	-3.3622426	-2.7097362	-1.0341868
H	-2.5996364	-2.6434113	-4.6635306

H	-3.8052113	-1.9062771	-3.5644612
H	-3.3853938	-3.6457109	-3.3933901
H	1.8372705	-2.1952719	-2.7983198
H	-0.0044037	1.7132656	-2.9646152
H	1.4176981	3.4716245	-3.9657769
H	2.9547317	2.9222793	-5.8798361
H	3.0411728	0.5668210	-6.7515830
H	1.6290680	-1.2001183	-5.7291927
H	-2.0195517	1.9767777	-3.2924357
H	-3.4753617	3.1896682	-1.6650785
H	-4.4486290	2.0013211	0.3059347
H	-4.1278042	-0.4787013	0.5688588
H	0.2285129	0.5377349	-0.3648320
H	-0.2064571	2.7044011	0.9494570
H	0.5333929	5.0522368	1.4612015
H	1.6955934	5.5522434	3.6281098
H	2.1210558	3.7078400	5.2736930
H	1.3978460	1.3722848	4.7531879
H	0.6564661	-2.5989012	1.8435722
H	2.7346658	-3.8162298	1.1752744
H	4.8823991	-2.5571133	0.8636266
H	4.9430319	-0.0784932	1.2569089
H	2.8780959	1.1284769	1.9742274
H	1.4961308	-1.3418326	4.5147630
H	0.7171307	-2.2269756	6.7214101
H	-1.6727365	-1.9342500	7.4220662
H	-3.2851581	-0.7551251	5.9032524
H	-2.5021969	0.1164397	3.6792708
C	1.8682618	0.0559925	-1.2538797
O	1.0647896	0.9829036	-0.7509122
O	2.9953059	0.6341432	-1.7099292
H	3.5175119	-0.0850776	-2.1190480

S4

79

SCF Energy = -2238.439514668

C	-1.6264444	0.4107451	-2.3129074
C	-1.6573389	1.0482925	-1.0543358
C	-2.8739101	1.1125279	-0.3434255
C	-4.0417011	0.5571238	-0.8898889
C	-4.0068610	-0.0638857	-2.1494628
C	-2.7976091	-0.1309849	-2.8598425
P	-0.0946563	1.6261943	-0.2786881
C	-0.6516630	3.0126769	0.8078218
C	-1.4451508	4.0679386	0.3115886
C	-1.8470595	5.1068831	1.1629128

C	-1.4563406	5.1044407	2.5144408
C	-0.6601874	4.0607616	3.0119122
C	-0.2587526	3.0184001	2.1600655
Pd	0.8969717	0.0026773	0.8894698
C	-0.0686909	-1.1152806	3.3544874
C	-1.1412045	-2.0838591	2.7720617
C	-0.6071491	-2.4058789	1.3692380
C	-1.6087002	-2.5591942	0.4492740
C	-2.9524980	-2.3088886	1.1357022
C	-2.5577317	-1.5706391	2.4470612
C	0.8590854	-2.3023530	1.4171283
C	1.8958484	-2.9479525	0.6962946
C	3.2284690	-2.7276088	1.0665967
C	3.5549419	-1.8485410	2.1203696
C	2.5457640	-1.2170143	2.8663042
C	1.1878715	-1.4662404	2.5520341
C	-1.5249838	-2.8192086	-0.9906120
C	-2.6334561	-3.3737588	-1.6778916
C	-2.5794990	-3.5989064	-3.0604178
C	-1.4256440	-3.2672224	-3.7919147
C	-0.3267095	-2.6984171	-3.1239894
C	-0.3753140	-2.4781089	-1.7425573
C	-1.1718252	-3.3643268	3.6367434
O	-3.7206589	-3.5098187	1.3289497
O	4.1878196	0.2908320	-0.2535561
C	0.7994454	2.5127744	-1.6223151
C	2.1983686	2.6278224	-1.4882452
C	2.9409386	3.3353207	-2.4459272
C	2.2940540	3.9266508	-3.5439050
C	0.8998159	3.8118697	-3.6814213
C	0.1516709	3.1092963	-2.7240235
H	-3.5962972	-1.6643301	0.5032102
H	-3.3078026	-1.7353553	3.2455603
H	-2.5084048	-0.4836155	2.2277800
H	-0.3691361	-0.0556009	3.1955314
H	0.0929415	-1.2472799	4.4445773
H	-1.8660071	-4.1175393	3.2153538
H	-1.5163947	-3.1281256	4.6643879
H	-0.1651164	-3.8253923	3.7052143
H	-3.0827458	-4.2169801	1.5430548
H	-3.5304198	-3.6435151	-1.1012832
H	-3.4487551	-4.0386935	-3.5734451
H	-1.3853085	-3.4465144	-4.8772258
H	0.5759248	-2.4071877	-3.6829780
H	0.4707800	-1.9901687	-1.2441891
H	1.9505961	-0.3242461	-0.8129742

H	2.8039823	-0.5641020	3.7135388
H	4.6097779	-1.6503794	2.3563931
H	4.0355609	-3.2229607	0.5068819
H	1.6487459	-3.6213840	-0.1355405
H	2.7094318	2.1436763	-0.6402777
H	4.0330306	3.4123973	-2.3350473
H	2.8777881	4.4746150	-4.2993254
H	0.3902830	4.2708923	-4.5425010
H	-0.9378349	3.0119061	-2.8434291
H	-1.7534151	4.0744961	-0.7445454
H	-2.4681693	5.9261810	0.7699988
H	-1.7727256	5.9221835	3.1797174
H	-0.3475142	4.0572693	4.0670938
H	0.3741911	2.1939762	2.5292226
H	-2.9077340	1.6040818	0.6402003
H	-4.9858264	0.6135242	-0.3269434
H	-4.9211498	-0.5039280	-2.5744289
H	-2.7562206	-0.6339667	-3.8362521
H	-0.6793381	0.3323062	-2.8657033
C	3.8368827	-0.3720713	-1.2072363
O	4.7211528	-0.9173935	-2.0779544
O	2.5718027	-0.6656993	-1.5628652
H	4.2049422	-1.4072688	-2.7498466

Optimized Geometries(TS-BXne-k)

R3
79
SCF Energy = -4548.281800943

C	0.0694403	-6.5292970	1.4698277
C	-0.4811696	-5.3643768	0.8836040
C	-1.6055149	-5.5109707	0.0334491
C	-2.1330957	-6.7758986	-0.2500537
C	-1.5578015	-7.9275233	0.3177843
C	-0.4585400	-7.7967162	1.1816735
C	0.0484562	-4.0297430	1.2142741
Pd	-0.2090394	0.2751202	-0.9184876
P	-0.0700514	2.4206688	0.2365228
C	0.1993895	-2.9246546	0.4162098
Br	-0.3643153	1.6304226	-3.1365083
C	0.1191619	-2.8323937	-1.0500865
C	0.4168019	-3.9987120	-1.8072271
C	0.2958163	-4.0314189	-3.1964919

C	-0.1307448	-2.8772617	-3.8713467
C	-0.3641587	-1.6963549	-3.1506675
C	-0.1958566	-1.6264580	-1.7494533
C	0.4813503	-3.7193455	2.6476930
O	-0.2382140	-4.4014335	3.6635677
C	0.3701126	-2.1818623	2.7036787
C	0.5412724	-1.6862892	1.2373479
C	-0.4823986	-0.5931592	0.9406988
C	1.9887545	-1.2215290	0.9759425
H	1.5398415	-4.0385850	2.7953866
H	1.0860764	-1.7065476	3.4027133
H	-0.6530394	-1.9460586	3.0658790
H	-1.5103683	-1.0047326	0.9827977
H	-0.3978442	0.2140474	1.6968529
H	2.2422479	-0.3433279	1.5985549
H	2.1348601	-0.9450599	-0.0902786
H	2.7102652	-2.0312072	1.2067756
H	-1.1770473	-4.3971534	3.3936023
H	-2.0601340	-4.6112337	-0.4065253
H	-3.0052891	-6.8655005	-0.9156761
H	-1.9733809	-8.9221233	0.0955262
H	-0.0088338	-8.6905726	1.6406220
H	0.9209904	-6.4370955	2.1584218
H	-1.5301356	0.5140099	-1.6714570
H	-0.6487869	-0.7928773	-3.7067454
H	-0.2580196	-2.8792771	-4.9651880
H	0.5309872	-4.9543782	-3.7481186
H	0.7521397	-4.8969118	-1.2712926
C	0.0349907	4.0613145	-0.5870838
C	1.4708586	2.2969213	1.2190590
C	-1.4257436	2.7410800	1.4360537
C	-1.3548705	3.8403748	2.3193810
C	-2.4187820	4.1105166	3.1911420
C	-3.5668064	3.2979341	3.1758251
C	-3.6505357	2.2180237	2.2829580
C	-2.5829611	1.9387275	1.4143934
H	-0.4679767	4.4923762	2.3131347
H	-2.3570075	4.9662777	3.8803060
H	-4.4028144	3.5149303	3.8578275
H	-4.5523383	1.5880665	2.2590435
H	-2.6439159	1.0975830	0.7086042
C	1.1093757	4.9518890	-0.4014406
C	1.0971431	6.2079876	-1.0315353
C	0.0135685	6.5823836	-1.8404926
C	-1.0648415	5.6979618	-2.0185914
C	-1.0547820	4.4413855	-1.4001415

H	1.9572248	4.6720818	0.2397100
H	1.9416354	6.8978985	-0.8827578
H	0.0072324	7.5660519	-2.3338932
H	-1.9168433	5.9846477	-2.6529966
H	-1.8943731	3.7480170	-1.5519208
C	1.4855797	2.1416574	2.6191505
C	2.7002083	1.9145573	3.2883517
C	3.9036134	1.8467546	2.5686695
C	3.8924812	1.9944307	1.1700139
C	2.6827368	2.2054579	0.4952286
H	0.5462594	2.1914222	3.1884939
H	2.7024675	1.7874994	4.3813327
H	4.8524436	1.6680083	3.0962074
H	4.8306354	1.9278539	0.5991934
H	2.6719137	2.2867999	-0.6034764

R4

79

SCF Energy = -4548.285564658

C	-0.9247499	5.2606305	0.4139865
C	-0.6550613	3.8981730	0.0910293
C	-0.5909414	3.5067189	-1.2687375
C	-0.7122748	4.4403124	-2.3031178
C	-0.8900181	5.7970050	-1.9908121
C	-1.0103546	6.1905701	-0.6483096
C	-0.3100875	2.9271615	1.1391465
C	0.6849402	1.9953080	1.0798722
C	1.6453763	1.7474818	-0.0151313
C	1.8299820	0.4445387	-0.5350756
C	2.7789499	0.2045966	-1.5428899
C	3.5591983	1.2586084	-2.0438767
C	3.3865820	2.5571318	-1.5310418
C	2.4418743	2.7998182	-0.5257031
Br	-2.9532129	7.6758742	1.6681455
C	-0.8893975	3.0393535	2.5449477
C	-2.4254828	3.0897128	2.5947988
C	-0.2602077	4.2691209	3.2024764
C	-0.3537445	1.7414804	3.2257172
C	0.8891663	1.3231140	2.4351173
O	0.9881371	-0.1008166	2.4062591
H	1.8194924	1.7496383	2.8903138
H	-0.1664920	1.8648758	4.3106899
H	-1.0983564	0.9286610	3.0994301
H	0.8484049	4.2375263	3.1802812
H	-0.6102517	4.3482953	4.2538393
H	-2.8619206	2.1829962	2.1303743

H	-2.8220700	3.9751110	2.0623169
H	-2.7746500	3.1434981	3.6471776
H	1.8502385	-0.3161204	2.0021722
H	1.1945405	-0.3714436	-0.1602068
H	2.9024129	-0.8127009	-1.9453829
H	4.3006174	1.0706818	-2.8353537
H	3.9959511	3.3878853	-1.9188153
H	2.3025736	3.8144428	-0.1236189
H	-0.4239763	2.4460262	-1.5039936
H	-0.6596078	4.1093777	-3.3514510
H	-0.9701158	6.5502620	-2.7897448
H	-1.2146389	7.2482394	-0.4229756
H	-2.2158877	6.0765177	1.3619822
Pd	-0.8503571	6.0551815	2.3544972
P	-0.4088049	7.1025355	4.4090496
C	-0.4742639	8.9292164	4.2683117
C	-0.1090911	9.5073571	3.0344632
H	0.1610697	8.8575314	2.1872889
C	-0.1116547	10.9019221	2.8836923
H	0.1714889	11.3470726	1.9182344
C	-0.4943338	11.7235521	3.9570164
H	-0.5076644	12.8172311	3.8351341
C	-0.8722908	11.1489821	5.1825295
H	-1.1825643	11.7909155	6.0208124
C	-0.8617544	9.7547455	5.3415844
H	-1.1671647	9.3067140	6.2986018
C	1.2533565	6.7655945	5.1139340
C	1.5064215	5.5478514	5.7855222
H	0.6850927	4.8440176	5.9807309
C	2.8034190	5.2375861	6.2200803
H	2.9871312	4.2883407	6.7456655
C	3.8611196	6.1328272	5.9884080
H	4.8776815	5.8868503	6.3303293
C	3.6142263	7.3451066	5.3236261
H	4.4362133	8.0545653	5.1445488
C	2.3186644	7.6623097	4.8875395
H	2.1319335	8.6153590	4.3711056
C	-1.5875787	6.6583023	5.7383959
C	-1.2516718	6.7309506	7.1070173
H	-0.2378510	7.0331189	7.4095871
C	-2.2084431	6.4050682	8.0809196
H	-1.9423834	6.4597523	9.1474274
C	-3.5004098	6.0084779	7.6953839
H	-4.2470391	5.7496721	8.4614419
C	-3.8375092	5.9385222	6.3331077
H	-4.8478449	5.6278935	6.0276933

C	-2.8852618	6.2593431	5.3541269
H	-3.1410217	6.2119579	4.2836649

S3

79

SCF Energy = -4548.291681654

C	-1.9841859	-0.2253298	-2.0256696
C	-1.3902658	-1.1163982	-2.9556410
C	-1.9369997	-1.3004562	-4.2366693
C	-3.1021564	-0.6029870	-4.5982921
C	-3.7011494	0.2777958	-3.6836094
C	-3.1435695	0.4718481	-2.4039811
C	-0.1522861	-1.7341284	-2.4343344
C	1.1190209	-1.2851551	-2.6184804
C	1.5947462	-0.2053113	-3.5124170
C	0.8435781	0.9785046	-3.7152555
C	1.3460222	2.0108237	-4.5208826
C	2.5996161	1.8842998	-5.1417982
C	3.3594933	0.7189310	-4.9412692
C	2.8652768	-0.3108105	-4.1286060
Br	-1.1669671	2.5750684	-0.2628390
C	-0.2769171	-2.7089376	-1.2519290
C	-0.8779987	-4.0540648	-1.7110756
C	-1.1997513	-2.0824651	-0.1834093
C	1.2074146	-2.8661844	-0.7993558
C	1.9776600	-1.7114821	-1.4414885
O	1.9895265	-0.5723379	-0.5329751
H	3.0309755	-1.9711674	-1.6884085
H	1.3305256	-2.8711988	0.2993115
H	1.6154290	-3.8221491	-1.1840822
H	-0.9474570	-2.4532656	0.8266561
H	-2.2640885	-2.2936629	-0.3944821
H	-0.2402246	-4.5310888	-2.4839144
H	-1.8882719	-3.9019520	-2.1416025
H	-0.9691332	-4.7529131	-0.8538557
H	2.0040314	0.2284910	-1.0986105
H	-0.1288167	1.0971535	-3.2186924
H	0.7509897	2.9267121	-4.6552368
H	2.9889736	2.6959051	-5.7751933
H	4.3446394	0.6124789	-5.4207685
H	3.4635192	-1.2225507	-3.9763173
H	-1.4394419	-1.9768817	-4.9485230
H	-3.5381760	-0.7419480	-5.5992956
H	-4.6106534	0.8302979	-3.9677279
H	-3.6077549	1.1966961	-1.7183159
H	-2.1345015	0.8922566	0.1721728

Pd	-0.9467652	-0.0141331	-0.2494157
P	0.0671617	0.0916600	1.9537154
C	-1.2110686	0.1769839	3.2765240
C	-2.5783677	0.2150319	2.9469348
H	-2.8779488	0.1982567	1.8879349
C	-3.5520711	0.2570328	3.9592271
H	-4.6182520	0.2862188	3.6891594
C	-3.1635237	0.2577586	5.3074347
H	-3.9254807	0.2904294	6.1009733
C	-1.7982709	0.2102115	5.6448087
H	-1.4905165	0.2046293	6.7014466
C	-0.8264678	0.1660955	4.6364971
H	0.2410052	0.1202947	4.9007352
C	1.1108891	1.5776715	2.2433475
C	2.3142833	1.7423914	1.5210812
H	2.6568166	0.9504836	0.8412764
C	3.0633868	2.9203716	1.6530561
H	4.0017936	3.0313489	1.0887618
C	2.6124300	3.9586113	2.4844138
H	3.1965538	4.8865206	2.5781538
C	1.4037939	3.8113376	3.1821641
H	1.0312333	4.6260038	3.8214507
C	0.6545412	2.6309424	3.0628770
H	-0.2991522	2.5381142	3.5997312
C	1.0304775	-1.3710041	2.5283006
C	2.4350516	-1.4511749	2.4563311
H	3.0222812	-0.5793731	2.1444270
C	3.0940800	-2.6463078	2.7830066
H	4.1921744	-2.6909059	2.7250315
C	2.3627013	-3.7784580	3.1775320
H	2.8830981	-4.7160883	3.4242601
C	0.9631424	-3.7024869	3.2663132
H	0.3793670	-4.5778819	3.5886197
C	0.3009415	-2.5071908	2.9490255
H	-0.7934318	-2.4514016	3.0460680

S4

79

SCF Energy = -4548.273234355

C	1.3518724	3.8001631	-1.8728915
C	0.5506142	3.8974911	-0.7010092
C	-0.7131972	4.5466613	-0.8009902
C	-1.1352253	5.0175444	-2.0671656
C	-0.3376931	4.8741504	-3.2133659
C	0.9149813	4.2507442	-3.1168459
C	1.1239543	3.3680159	0.5450862

C	2.0035326	2.3196277	0.6697652
C	2.4098407	1.3170344	-0.3390461
C	3.7459291	0.8489152	-0.4022001
C	4.1234882	-0.1209630	-1.3456364
C	3.1786719	-0.6498862	-2.2398446
C	1.8455985	-0.2042271	-2.1789756
C	1.4650854	0.7615222	-1.2391303
Br	-4.0121531	5.7255016	-0.7204922
C	0.8145872	4.0424571	1.8825715
C	1.3528854	5.4874615	1.9704686
C	-0.6997122	4.0309281	2.1188996
C	1.5679914	3.1075219	2.8950118
C	2.6029637	2.3127866	2.0677976
O	3.9261831	2.8814508	2.0711956
H	2.7519698	1.2873884	2.4643277
H	2.0664036	3.6640600	3.7132290
H	0.8613092	2.3891357	3.3608079
H	-1.0792713	2.9891728	2.0798656
H	-0.9443253	4.4811923	3.1001889
H	2.4570807	5.5192265	1.8745045
H	1.0878783	5.9322627	2.9519208
H	0.9205853	6.1281687	1.1758773
H	3.8994381	3.6571270	1.4769384
H	4.4880353	1.2735824	0.2900821
H	5.1690885	-0.4638071	-1.3858954
H	3.4756660	-1.4100124	-2.9790208
H	1.0953743	-0.6160142	-2.8718258
H	0.4203721	1.1019223	-1.1975113
H	-2.5727967	3.7115480	0.3859961
H	-2.1163866	5.4993195	-2.1629266
H	-0.7019842	5.2483985	-4.1840002
H	1.5479924	4.1052662	-4.0052491
H	2.3446057	3.3393819	-1.7858945
Pd	-1.9633676	5.0418184	0.7706462
P	-3.2639139	6.0103567	2.8020128
C	-2.0677386	6.5331608	4.1115052
C	-1.9649866	5.8697246	5.3527765
H	-2.6576937	5.0520114	5.5985086
C	-0.9802493	6.2491398	6.2813628
H	-0.9111633	5.7235926	7.2461220
C	-0.0927050	7.2952620	5.9857067
H	0.6750592	7.5914621	6.7169069
C	-0.1881661	7.9612622	4.7508523
H	0.5058801	8.7815475	4.5133233
C	-1.1613923	7.5777981	3.8150481
H	-1.2164933	8.0994033	2.8463058

C	-4.3068702	4.7549043	3.6482740
C	-5.3282095	5.1858155	4.5212843
H	-5.4955105	6.2625238	4.6691853
C	-6.1343577	4.2492382	5.1823775
H	-6.9299589	4.5987063	5.8574116
C	-5.9293037	2.8749198	4.9702864
H	-6.5736038	2.1409066	5.4773505
C	-4.9127394	2.4402307	4.1039962
H	-4.7568043	1.3644424	3.9329091
C	-4.1005322	3.3759709	3.4409280
H	-3.3102689	3.0363159	2.7562528
C	-4.4365502	7.4414031	2.6647397
C	-4.3584342	8.6275024	3.4308100
H	-3.6405990	8.7209004	4.2595392
C	-5.1995545	9.7147277	3.1242599
H	-5.1777525	10.6212740	3.7483671
C	-6.0425817	9.6666417	2.0005616
H	-6.5935799	10.5649300	1.6802835
C	-6.1705167	8.4682684	1.2824904
H	-6.8136359	8.4134684	0.3896661
C	-5.4298865	7.3408201	1.6635815
H	-5.5801036	6.3894648	1.1410263

Optimized Geometries(BXnk)

R3
75
SCF Energy = -4548.296931013

C	0.5663550	-6.7761834	0.7332637
C	-0.0769977	-5.5862358	0.3160774
C	-1.1176754	-5.6875814	-0.6401963
C	-1.4733862	-6.9260729	-1.1872025
C	-0.8058068	-8.0969562	-0.7840694
C	0.2109180	-8.0158595	0.1813145
C	0.2715981	-4.2884483	0.9203049
Pd	-0.2532659	0.2842652	-0.4591179
P	-0.1494962	2.3724357	0.6548743
C	0.3522478	-3.0506457	0.3379387
Br	-3.1886601	1.0679001	-1.7500664
C	0.3419412	-2.7009649	-1.0917746
C	0.7706481	-3.6295937	-2.0767108
C	0.7311797	-3.3150480	-3.4386624
C	0.2516694	-2.0615647	-3.8595319

C	-0.1465854	-1.1191688	-2.8969050
C	-0.0601666	-1.4087735	-1.5181847
C	0.5643943	-4.1985438	2.4174932
O	-0.1452389	-5.1152206	3.2345791
C	0.2818509	-2.7126402	2.7230348
C	0.5460585	-1.9500975	1.3887745
C	-0.4867170	-0.8407695	1.2403502
C	1.9846052	-1.3926337	1.3513372
H	1.6387880	-4.4325340	2.6041262
H	0.8707954	-2.3097352	3.5702402
H	-0.7923111	-2.6386709	2.9958755
H	-1.5163549	-1.2494917	1.1965092
H	-0.4020056	-0.1128656	2.0736222
H	2.1166584	-0.5933079	2.1075300
H	2.2089635	-0.9597727	0.3553040
H	2.7260603	-2.1919904	1.5525596
H	-1.0599613	-5.1473961	2.8929217
H	-1.6466367	-4.7743691	-0.9500605
H	-2.2837807	-6.9803848	-1.9301583
H	-1.0865375	-9.0708140	-1.2131810
H	0.7304468	-8.9280972	0.5125786
H	1.3534840	-6.7255442	1.4986636
H	-1.9381030	0.4688751	-0.9737682
H	-0.5295791	-0.1391422	-3.2343320
H	0.1927473	-1.8151200	-4.9310079
H	1.0706275	-4.0552275	-4.1791534
H	1.1467673	-4.6113507	-1.7570858
C	0.1611218	3.8535541	-0.3845335
C	1.2814498	2.2748547	1.7980158
C	-1.5572407	2.8710855	1.7207353
C	-1.5649633	4.1258568	2.3665679
C	-2.6433068	4.4852452	3.1867409
C	-3.7211605	3.5983127	3.3619315
C	-3.7204143	2.3540264	2.7124369
C	-2.6419153	1.9892053	1.8902377
H	-0.7267098	4.8241352	2.2204407
H	-2.6470118	5.4650977	3.6877839
H	-4.5691268	3.8844569	4.0025317
H	-4.5680714	1.6636492	2.8358990
H	-2.6476888	1.0251153	1.3632864
C	1.0925894	4.8554124	-0.0420853
C	1.2544888	5.9745109	-0.8742927
C	0.4888944	6.1008638	-2.0454947
C	-0.4418417	5.1044798	-2.3863342
C	-0.6058000	3.9803554	-1.5635372
H	1.6959098	4.7571046	0.8726149

H	1.9838868	6.7533642	-0.6044266
H	0.6197508	6.9788042	-2.6961308
H	-1.0441759	5.1990553	-3.3023517
H	-1.3416315	3.2019225	-1.8272943
C	1.1113547	2.1273835	3.1889132
C	2.2236247	1.8814307	4.0122428
C	3.5091249	1.7900182	3.4565922
C	3.6830741	1.9371402	2.0684333
C	2.5757513	2.1651750	1.2412684
H	0.1062403	2.2036334	3.6289948
H	2.0809925	1.7623859	5.0969101
H	4.3781027	1.5984164	4.1037226
H	4.6873822	1.8581871	1.6258901
H	2.7125352	2.2490724	0.1517503

R4

75

SCF Energy = -4548.295910824

C	-0.5597981	5.3403687	0.3150255
C	-0.4100134	3.9794052	-0.0455028
C	-0.2364233	3.6362561	-1.4057995
C	-0.2194280	4.6303695	-2.3942826
C	-0.3804819	5.9806736	-2.0394011
C	-0.5546571	6.3305211	-0.6869038
C	-0.4512084	2.9703379	1.0225121
C	0.3538648	1.8887706	1.2069545
C	1.5094362	1.4841920	0.3825118
C	1.6640666	0.1439872	-0.0461975
C	2.7824873	-0.2405402	-0.8034463
C	3.7643397	0.7033620	-1.1446986
C	3.6210997	2.0381505	-0.7249192
C	2.5073085	2.4247633	0.0316933
Br	-3.3597939	7.7546121	1.9115231
C	-1.4204607	3.1805775	2.1868188
C	-2.8638086	3.4554190	1.7359585
C	-0.9001872	4.3119342	3.0685091
C	-1.2995672	1.8237531	2.9504344
C	0.0451000	1.2077512	2.5395384
O	-0.0757621	-0.2149905	2.4962171
H	0.8537641	1.4843216	3.2633000
H	-1.4206958	1.9242455	4.0471411
H	-2.0881729	1.1343470	2.5849953
H	0.0775884	4.0565467	3.5312717
H	-1.6276142	4.5914311	3.8574633
H	-3.2288745	2.6456431	1.0733487
H	-2.9365441	4.4135470	1.1868436

H	-3.5362670	3.5159722	2.6163549
H	0.8275748	-0.5758639	2.4231504
H	0.8748632	-0.5832719	0.1940032
H	2.8815538	-1.2846188	-1.1384982
H	4.6391332	0.4016708	-1.7406718
H	4.3863844	2.7839280	-0.9897558
H	2.3923521	3.4682421	0.3610832
H	-0.1235119	2.5770549	-1.6813954
H	-0.0943296	4.3489589	-3.4509584
H	-0.3900518	6.7623334	-2.8149239
H	-0.7074484	7.3927179	-0.4236414
H	-2.1464365	6.7501468	2.0195513
Pd	-0.4801945	6.1130090	2.1666967
P	-0.1696179	7.2324979	4.2466841
C	-0.5727010	9.0194600	4.2190245
C	-0.2429449	9.7390649	3.0516486
H	0.2283306	9.2182673	2.2021709
C	-0.5238149	11.1090766	2.9647378
H	-0.2697107	11.6629280	2.0487201
C	-1.1463984	11.7672310	4.0393871
H	-1.3779920	12.8405794	3.9669323
C	-1.4828536	11.0528039	5.2007792
H	-1.9765204	11.5652147	6.0403633
C	-1.1972727	9.6812269	5.2941907
H	-1.4726560	9.1187192	6.1986447
C	1.5626266	7.1693745	4.8551572
C	2.4141642	6.1673171	4.3455775
H	2.0352771	5.4752145	3.5763877
C	3.7366464	6.0645057	4.8057813
H	4.3964024	5.2811106	4.4034855
C	4.2161869	6.9669254	5.7693393
H	5.2543385	6.8902477	6.1265082
C	3.3736438	7.9750212	6.2710456
H	3.7518371	8.6877672	7.0195140
C	2.0507308	8.0788549	5.8162585
H	1.3929583	8.8724552	6.2020906
C	-1.1644021	6.5466294	5.6244717
C	-0.5757484	5.9201419	6.7400889
H	0.5188825	5.8998221	6.8451780
C	-1.3881344	5.3189733	7.7164532
H	-0.9225420	4.8298037	8.5854706
C	-2.7854829	5.3415046	7.5849018
H	-3.4189455	4.8688765	8.3507052
C	-3.3743329	5.9636504	6.4691553
H	-4.4689369	5.9788874	6.3570651
C	-2.5716240	6.5580216	5.4859106

H	-3.0342798	7.0259899	4.6008673
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S3

75

SCF Energy = -4548.301812355

C	-2.2931475	0.4072712	-1.8873351
C	-1.5346604	-0.3033725	-2.8508725
C	-1.6790858	-0.0222174	-4.2254093
C	-2.6093972	0.9405432	-4.6453416
C	-3.3843065	1.6275345	-3.6949984
C	-3.2199378	1.3709564	-2.3203337
C	-0.6265337	-1.3448483	-2.3315925
C	0.7222763	-1.4731218	-2.4618018
C	1.6692396	-0.5085188	-3.0395285
C	1.4300564	0.8858305	-2.9567742
C	2.3782557	1.8042499	-3.4210591
C	3.5964159	1.3595770	-3.9671056
C	3.8542945	-0.0182811	-4.0493666
C	2.9011549	-0.9424626	-3.5912290
Br	-1.7420792	2.7844548	0.6244301
C	-1.2416062	-2.4645023	-1.4775358
C	-2.0598956	-3.4149540	-2.3809907
C	-2.1527926	-1.8654775	-0.3842569
C	0.0206337	-3.1648215	-0.9029020
C	1.2104976	-2.7532102	-1.7870419
O	2.3653445	-2.5671496	-0.9613664
H	1.4331602	-3.5322153	-2.5604685
H	0.2381135	-2.7805263	0.1100981
H	-0.1020093	-4.2617453	-0.8166662
H	-2.0517672	-2.4089836	0.5749036
H	-3.2154499	-1.8432414	-0.6878778
H	-1.4124858	-3.8906600	-3.1467427
H	-2.8615645	-2.8587056	-2.9072845
H	-2.5315638	-4.2180533	-1.7780293
H	3.0402935	-2.1222840	-1.5126603
H	0.5009725	1.2436878	-2.4918210
H	2.1723557	2.8819557	-3.3364569
H	4.3431646	2.0851452	-4.3233986
H	4.8011962	-0.3786424	-4.4798796
H	3.1030061	-2.0211398	-3.6947707
H	-1.0615462	-0.5671165	-4.9561258
H	-2.7336313	1.1536563	-5.7180681
H	-4.1194205	2.3788041	-4.0242824
H	-3.8076353	1.9502233	-1.5917883
H	-2.5662399	1.3433492	0.5501137
Pd	-1.5886256	0.1020316	-0.0045411

P	-0.2879332	-0.1961561	1.9879906
C	-0.8846922	0.4144649	3.6131371
C	-2.1881450	0.9303439	3.7386948
H	-2.8372652	0.9873929	2.8535258
C	-2.6541707	1.3697770	4.9888077
H	-3.6741172	1.7724024	5.0797766
C	-1.8204795	1.2964819	6.1156100
H	-2.1856673	1.6430919	7.0943208
C	-0.5197874	0.7740222	5.9961778
H	0.1326210	0.7085877	6.8801148
C	-0.0538357	0.3287608	4.7515251
H	0.9587687	-0.0929244	4.6582392
C	1.2216985	0.7700545	1.6068690
C	1.9884636	0.3735590	0.4876232
H	1.7702737	-0.5646399	-0.0457585
C	3.0567996	1.1695386	0.0509481
H	3.6417012	0.8534573	-0.8257237
C	3.3571380	2.3725470	0.7113882
H	4.1874281	3.0029073	0.3585570
C	2.5877460	2.7744572	1.8159868
H	2.8133177	3.7205244	2.3312551
C	1.5209290	1.9798277	2.2645673
H	0.9085723	2.3097411	3.1157796
C	0.2737685	-1.8885782	2.4283059
C	1.6070191	-2.3276879	2.3246576
H	2.3951521	-1.6305277	2.0112427
C	1.9263016	-3.6682387	2.5937814
H	2.9685901	-4.0055229	2.4937488
C	0.9242324	-4.5742706	2.9736226
H	1.1782118	-5.6257660	3.1756499
C	-0.4061841	-4.1353665	3.0963950
H	-1.1955120	-4.8389454	3.4014273
C	-0.7317477	-2.8003385	2.8225479
H	-1.7734537	-2.4560261	2.9218220

S4

75

SCF Energy = -4548.299602416

C	1.2976302	4.0375188	-1.7661649
C	0.5110921	3.9653785	-0.5869444
C	-0.7515330	4.6115029	-0.5768036
C	-1.2412314	5.2102983	-1.7569140
C	-0.4609907	5.2501988	-2.9247284
C	0.8219241	4.6740488	-2.9171935
C	1.0052041	3.2686805	0.6113643
C	1.8706296	2.2068944	0.6861480

C	2.3938490	1.3497875	-0.3938003
C	3.7313147	0.8866873	-0.3582985
C	4.2207895	0.0369271	-1.3619522
C	3.3845162	-0.3754214	-2.4121489
C	2.0475620	0.0613575	-2.4461679
C	1.5558470	0.9111711	-1.4479937
Br	-4.6623659	3.8590828	-0.3881781
C	0.5597142	3.7387454	1.9999249
C	1.1064362	5.1413661	2.3379321
C	-0.9594574	3.6954245	2.1221470
C	1.1753479	2.6497449	2.9375346
C	2.3035596	1.9822915	2.1276845
O	3.6067334	2.5432022	2.3697300
H	2.4133461	0.9071382	2.3785520
H	1.5481759	3.0692070	3.8924746
H	0.4098731	1.8843778	3.1806921
H	-1.3629742	2.7127708	1.8046412
H	-1.2745570	3.9204116	3.1619024
H	2.2149330	5.1393871	2.3654296
H	0.7417312	5.4740252	3.3300163
H	0.7785819	5.8861088	1.5848258
H	3.6250239	3.3949314	1.8905873
H	4.3802254	1.2170470	0.4663616
H	5.2662353	-0.3060293	-1.3222471
H	3.7692679	-1.0423793	-3.1986736
H	1.3793838	-0.2704170	-3.2556587
H	0.5072099	1.2417575	-1.4711402
H	-3.2700952	4.1439093	0.3174529
H	-2.2524803	5.6555759	-1.7741214
H	-0.8528428	5.7316562	-3.8340659
H	1.4529082	4.7156883	-3.8179864
H	2.3006845	3.5881290	-1.7676431
Pd	-1.9269493	5.0970063	0.9758432
P	-3.1883975	6.0117162	2.7613774
C	-1.9714152	6.6063987	3.9977809
C	-1.7413214	5.9158366	5.2042030
H	-2.3922662	5.0754686	5.4867689
C	-0.6810713	6.2989295	6.0437500
H	-0.5048971	5.7505946	6.9814245
C	0.1473652	7.3755345	5.6911475
H	0.9758293	7.6738620	6.3508584
C	-0.0800955	8.0685466	4.4881519
H	0.5708524	8.9084421	4.2026644
C	-1.1242406	7.6793326	3.6391031
H	-1.2795183	8.2042321	2.6835355
C	-4.3048192	4.9045436	3.7064336

C	-5.1247520	5.4122683	4.7366614
H	-5.1103680	6.4876951	4.9708411
C	-5.9632036	4.5483613	5.4546203
H	-6.6030326	4.9474670	6.2561940
C	-5.9922419	3.1762968	5.1452129
H	-6.6552353	2.5008361	5.7068816
C	-5.1847076	2.6706487	4.1145053
H	-5.2150781	1.6006914	3.8604020
C	-4.3427594	3.5321405	3.3926984
H	-3.7247089	3.1437388	2.5714254
C	-4.2355731	7.4683892	2.3731086
C	-4.2875135	8.6194937	3.1861727
H	-3.6601758	8.6860775	4.0875267
C	-5.1352541	9.6835843	2.8394624
H	-5.1717292	10.5808356	3.4759090
C	-5.9342150	9.6038242	1.6866198
H	-6.5964229	10.4405862	1.4173426
C	-5.8852578	8.4560881	0.8769933
H	-6.5094067	8.3886171	-0.0267525
C	-5.0371201	7.3906136	1.2130887
H	-5.0047022	6.4866196	0.5816677

Optimized Geometries(TS-BXnc-d-6)

R4
75
SCF Energy = -4548.292553288

C	3.0976205	2.3606904	-0.1368221
C	1.7782822	1.8620946	-0.0031895
C	1.5361399	0.5039782	-0.3202339
C	2.5723153	-0.3257604	-0.7677757
C	3.8741886	0.1845024	-0.9090052
C	4.1312066	1.5289357	-0.5901641
C	0.6674706	2.7405011	0.4457533
Pd	-1.4369670	4.6731587	0.1332660
P	-1.9536554	6.8980394	0.5477039
C	-0.5170977	2.8014958	-0.2448018
Br	-0.5360131	5.5505453	-2.0675337
C	-0.8225033	2.1411833	-1.5273202
C	0.0989432	2.2552771	-2.5993032
C	-0.1588216	1.6471877	-3.8321236
C	-1.3441306	0.9184400	-4.0335214
C	-2.2747474	0.8135701	-2.9880467

C	-2.0199404	1.4243815	-1.7507378
C	0.8945237	3.5896298	1.7045876
O	2.0716735	3.2452741	2.4225736
C	-0.3234021	3.5632260	2.6809927
C	-1.6978298	3.7419585	2.0613018
C	-2.0841225	2.7431150	1.0881560
C	-2.7561629	4.3262881	2.9666710
H	1.0480828	4.6432827	1.3866927
H	-0.1463971	4.3430254	3.4503457
H	-0.2769666	2.5880276	3.2170333
H	-1.7400290	1.7018456	1.1810618
H	-3.1251393	2.7950279	0.7186455
H	-2.9458555	3.6245170	3.8108075
H	-3.7165034	4.4857436	2.4411323
H	-2.4435424	5.2906785	3.4098516
H	2.1793587	2.2758867	2.3633210
H	0.5161958	0.1051134	-0.2203218
H	2.3613807	-1.3783023	-1.0107331
H	4.6879965	-0.4651302	-1.2653270
H	5.1474660	1.9370159	-0.7012973
H	3.3016323	3.4118983	0.1073941
H	-2.7653000	1.3365453	-0.9487927
H	-3.2118939	0.2552050	-3.1354598
H	-1.5464690	0.4443037	-5.0059235
H	0.5694263	1.7542179	-4.6502342
H	1.0134361	2.8431205	-2.4514722
C	-2.8969497	7.8281801	-0.7257034
C	-0.3256163	7.7182533	0.7389421
C	-2.9192870	7.4218101	2.0345637
C	-2.3629472	8.0687675	3.1543108
C	-3.1711735	8.3880253	4.2596936
C	-4.5378304	8.0701554	4.2544280
C	-5.1018510	7.4394547	3.1306109
C	-4.2985822	7.1169165	2.0298408
H	-1.2967862	8.3356634	3.1634911
H	-2.7255573	8.8957242	5.1287058
H	-5.1674926	8.3205679	5.1214669
H	-6.1754906	7.1979732	3.1133218
H	-4.7437859	6.6275950	1.1488931
C	-3.1079549	9.2136351	-0.5581772
C	-3.8838801	9.9232749	-1.4861094
C	-4.4717354	9.2499933	-2.5713517
C	-4.2805811	7.8675031	-2.7266434
C	-3.4904432	7.1552059	-1.8102225
H	-2.6693614	9.7360941	0.3057864
H	-4.0366570	11.0055263	-1.3570782

H	-5.0845563	9.8067428	-3.2967066
H	-4.7408266	7.3369073	-3.5736298
H	-3.3085699	6.0792182	-1.9419812
C	0.5113839	7.2705512	1.7851206
C	1.8146196	7.7712577	1.9141036
C	2.2974300	8.7133311	0.9895702
C	1.4732518	9.1472319	-0.0613477
C	0.1666489	8.6506170	-0.1926908
H	0.1455214	6.5118274	2.4936390
H	2.4590875	7.4098453	2.7294214
H	3.3237137	9.0995953	1.0818718
H	1.8545718	9.8698243	-0.7985167
H	-0.4630900	8.9663954	-1.0358788

S4

75

SCF Energy = -4548.305081714

C	-1.9569223	3.4828322	-1.5936960
C	-1.0610529	2.5696816	-0.9926324
C	-0.7633267	1.3681640	-1.6831170
C	-1.3178926	1.1074448	-2.9425020
C	-2.1891059	2.0358621	-3.5380877
C	-2.5068400	3.2224803	-2.8559192
C	-0.5024615	2.7892431	0.3538142
C	0.7579613	2.4635903	0.7840470
C	1.8689939	2.2233144	-0.1721403
C	2.7843621	1.1621834	0.0137816
C	3.8201298	0.9405818	-0.9059331
C	3.9684757	1.7859640	-2.0182159
C	3.0766827	2.8574294	-2.2006122
C	2.0367208	3.0765243	-1.2885134
Br	-0.1923550	6.0325761	0.1628112
C	-1.3984390	2.5571004	2.9728233
C	-2.3090577	2.6448692	4.1707046
C	-1.9248737	2.1012404	1.7109097
C	0.0408758	2.1405004	3.2687469
C	1.1338586	2.5749325	2.2581246
O	1.6005160	3.9031120	2.5413378
H	2.0082151	1.9128247	2.4377203
H	0.3466020	2.5390663	4.2570046
H	0.0689491	1.0283552	3.3530060
H	-1.5823635	1.1566246	1.2627613
H	-2.9911339	2.2942534	1.4936301
H	-1.9211430	3.3358073	4.9426483
H	-2.3835290	1.6371884	4.6397446
H	-3.3325913	2.9628318	3.9000111

H	1.2166884	4.5087379	1.8625467
H	2.6691931	0.4868316	0.8760813
H	4.5156318	0.1009855	-0.7533600
H	4.7844547	1.6153138	-2.7369262
H	3.1980573	3.5362606	-3.0585100
H	1.3514675	3.9294251	-1.4090532
H	-0.0800228	0.6407128	-1.2211061
H	-1.0683825	0.1703184	-3.4632369
H	-2.6238668	1.8314400	-4.5283383
H	-3.1892103	3.9556922	-3.3122799
H	-2.1868621	4.4170854	-1.0640632
Pd	-1.2668879	4.2637879	1.6759409
P	-1.9819093	6.0716857	2.9755279
C	-0.6157751	7.2345833	3.3734380
C	0.6110486	6.6737886	3.7867319
H	0.7472879	5.5806549	3.7913398
C	1.6807283	7.5101668	4.1377508
H	2.6365032	7.0627638	4.4493539
C	1.5398528	8.9060931	4.0635607
H	2.3841311	9.5613452	4.3266816
C	0.3246967	9.4632641	3.6331200
H	0.2151409	10.5555851	3.5539357
C	-0.7536137	8.6324366	3.2897480
H	-1.6946856	9.0757794	2.9354373
C	-2.7652592	5.7901942	4.6225432
C	-2.0316025	5.9006563	5.8203552
H	-0.9885571	6.2481227	5.7931760
C	-2.6298706	5.5742442	7.0489006
H	-2.0471871	5.6669567	7.9780009
C	-3.9641586	5.1398443	7.0942352
H	-4.4312347	4.8867758	8.0579508
C	-4.7037181	5.0371699	5.9028218
H	-5.7523864	4.7040868	5.9305067
C	-4.1080299	5.3556783	4.6748354
H	-4.6912686	5.2718067	3.7447787
C	-3.2850628	7.0743158	2.1443617
C	-4.0277120	8.0290627	2.8755326
H	-3.8383417	8.1664003	3.9504670
C	-5.0166926	8.7933896	2.2390887
H	-5.5866051	9.5370845	2.8164963
C	-5.2806939	8.6065824	0.8711350
H	-6.0594872	9.2045940	0.3738070
C	-4.5512495	7.6535586	0.1428303
H	-4.7532359	7.5013964	-0.9280565
C	-3.5557842	6.8913009	0.7742814
H	-2.9645051	6.1614284	0.2044570

Optimized Geometries(BXnd-6)

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R4
75
SCF Energy = -4548.346498328
C      1.4502956   -2.8133518    2.3410726
C      0.3032353   -3.3039358    1.6714069
C      0.1683804   -4.7033644    1.5203184
C      1.1602572   -5.5778919    1.9851081
C      2.3095761   -5.0743597    2.6167680
C      2.4462248   -3.6874363    2.7965649
C     -0.7139650   -2.3547471    1.1500073
Pd    -0.8559851    0.3882988   -0.9942017
P      0.0564305    2.0315488    0.1894472
C     -1.2975765   -2.4975378   -0.0784961
Br     0.7574062    0.1749968   -2.8941422
C     -0.9075731   -3.5517958   -1.0570281
C      0.4070096   -3.5794348   -1.5700007
C      0.7770187   -4.5383001   -2.5224492
C     -0.1598867   -5.4809938   -2.9786342
C     -1.4756485   -5.4503398   -2.4876271
C     -1.8494438   -4.4848898   -1.5397673
C     -1.0013914   -1.1337013    2.0174429
O     -0.9399898   -1.4104866    3.4143024
C     -2.3151362   -0.4500011    1.6472297
C     -2.4815811   -0.2217185    0.1621380
C     -2.2532008   -1.4713625   -0.6530671
C     -3.7120926    0.5846753   -0.2066866
H     -0.1780388   -0.4069711    1.8382537
H     -2.4066384    0.4948154    2.2142835
H     -3.1534351   -1.1025195    1.9968418
H     -3.2046643   -1.9350375   -1.0098502
H     -1.8289826   -1.1862037   -1.6981445
H     -4.6399747    0.0790556    0.1513701
H     -3.8074953    0.7270666   -1.3023440
H     -3.6822447    1.5819008    0.2738595
H     -1.4250495   -2.2439250    3.5651638
H     -0.7278419   -5.1073847    1.0303218
H      1.0329474   -6.6630106    1.8521715
H      3.0906847   -5.7607159    2.9774600
H      3.3356301   -3.2798395    3.3012233
H      1.5673698   -1.7332618    2.4980981
H     -2.8798388   -4.4674841   -1.1502616
H     -2.2161463   -6.1821387   -2.8450262

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H	0.1328661	-6.2343138	-3.7256555
H	1.8034653	-4.5422212	-2.9186968
H	1.1313084	-2.8282866	-1.2251619
C	0.2298444	3.6555076	-0.6552762
C	1.7653484	1.5642116	0.6846903
C	-0.7571843	2.4530396	1.7783259
C	-0.2675088	1.9680820	3.0072890
C	-1.0120606	2.1479912	4.1838578
C	-2.2377451	2.8306415	4.1463184
C	-2.7199904	3.3388202	2.9260489
C	-1.9898879	3.1436185	1.7458092
H	0.6908904	1.4312606	3.0442359
H	-0.6322482	1.7396445	5.1315659
H	-2.8211044	2.9687870	5.0690192
H	-3.6770625	3.8810755	2.8927723
H	-2.3735368	3.5300801	0.7890386
C	0.2394122	4.8644448	0.0750864
C	0.4334603	6.0845183	-0.5908868
C	0.6192346	6.1061218	-1.9833620
C	0.6111887	4.9033539	-2.7092773
C	0.4147091	3.6787085	-2.0531020
H	0.0868993	4.8545828	1.1644052
H	0.4377802	7.0235557	-0.0167291
H	0.7683915	7.0646582	-2.5035419
H	0.7566751	4.9137610	-3.8000160
H	0.4182026	2.7295885	-2.6158833
C	2.1935763	0.2324117	0.5219944
C	3.4756518	-0.1509417	0.9459103
C	4.3368013	0.7954358	1.5235165
C	3.9166982	2.1292307	1.6750027
C	2.6350255	2.5155969	1.2566944
H	1.5183149	-0.4934543	0.0433889
H	3.7983747	-1.1947367	0.8178641
H	5.3442166	0.4965578	1.8509330
H	4.5940351	2.8749396	2.1180123
H	2.3120532	3.5613348	1.3699718

S4

75

SCF Energy = -4548.350277218

C	-0.4901984	-3.6114562	-2.3962359
C	-0.9875249	-3.9149441	-1.1075434
C	-1.3193986	-5.2528263	-0.8016171
C	-1.1551575	-6.2647215	-1.7573135
C	-0.6543310	-5.9563962	-3.0338984
C	-0.3210724	-4.6284399	-3.3481677

C	-1.1479832	-2.8354699	-0.0961607
C	-0.5612419	-2.8702619	1.1348583
C	0.3630377	-3.9563576	1.5538890
C	0.1768064	-4.6236939	2.7842198
C	1.0483457	-5.6477464	3.1851974
C	2.1322921	-6.0094285	2.3684062
C	2.3391648	-5.3383518	1.1507863
C	1.4627125	-4.3227995	0.7461528
Br	1.0786439	0.2923348	-2.5587425
C	-2.1857980	-0.5034203	0.3964952
C	-3.4693703	0.2744481	0.1737982
C	-1.9495181	-1.6434833	-0.5635617
C	-1.9095785	-0.8360050	1.8491175
C	-0.6436112	-1.6669185	2.0638731
O	0.5562973	-0.8978777	1.8960250
H	-0.6110731	-2.0095663	3.1181528
H	-1.8524030	0.0894072	2.4561785
H	-2.7780470	-1.4170196	2.2441684
H	-2.8801444	-1.9600816	-1.0871147
H	-1.3925752	-1.2471212	-1.5238864
H	-3.4635978	1.2133031	0.7591205
H	-4.3511311	-0.3158002	0.5168331
H	-3.6267361	0.5283151	-0.8935957
H	0.5373644	-0.5990541	0.9466225
H	-0.6760580	-4.3504648	3.4254605
H	0.8792374	-6.1670767	4.1409362
H	2.8189046	-6.8099667	2.6831922
H	3.1936544	-5.6063216	0.5109906
H	1.6265022	-3.7947927	-0.2039575
H	-1.7032272	-5.4922400	0.2009396
H	-1.4187618	-7.3028430	-1.5035774
H	-0.5215191	-6.7521201	-3.7826411
H	0.0849551	-4.3792463	-4.3403081
H	-0.1820920	-2.5811530	-2.6427917
Pd	-0.6063175	0.2715868	-0.7196771
P	-0.0735284	2.1874252	0.3061476
C	1.7401070	2.4545098	0.4651545
C	2.5458760	1.4755286	1.0876092
H	2.1020138	0.5608120	1.5042026
C	3.9324546	1.6627341	1.1785944
H	4.5488697	0.8937789	1.6678997
C	4.5319917	2.8102586	0.6340456
H	5.6222899	2.9465561	0.6956679
C	3.7358453	3.7747406	-0.0023738
H	4.1977365	4.6700634	-0.4452442
C	2.3458506	3.6005511	-0.0886557

H	1.7347527	4.3550652	-0.6024570
C	-0.7802236	2.4575769	1.9802561
C	-0.0807012	2.0665162	3.1398803
H	0.9485767	1.6938035	3.0641051
C	-0.7027184	2.1380132	4.3957685
H	-0.1455448	1.8293623	5.2930163
C	-2.0257559	2.5956984	4.5095474
H	-2.5106877	2.6466167	5.4960079
C	-2.7256637	2.9933066	3.3580042
H	-3.7598419	3.3611282	3.4371994
C	-2.1088762	2.9232901	2.1000240
H	-2.6595538	3.2441893	1.2037261
C	-0.6699698	3.6250791	-0.6666107
C	-0.8110798	4.8989326	-0.0731541
H	-0.5951498	5.0350851	0.9969873
C	-1.2238162	5.9918755	-0.8493636
H	-1.3344853	6.9820712	-0.3819029
C	-1.4912472	5.8230087	-2.2193503
H	-1.8161197	6.6822398	-2.8256778
C	-1.3393771	4.5595761	-2.8132333
H	-1.5380033	4.4245446	-3.8870072
C	-0.9300558	3.4600919	-2.0421004
H	-0.7841510	2.4696260	-2.5030106

Optimized Geometries(TS-BXnd-l)

R4
75
SCF Energy = -4548.331360442

C	2.3678473	3.7166993	0.9671423
C	1.4625940	2.6357020	0.8227082
C	1.9966885	1.3480513	0.5791301
C	3.3780166	1.1532620	0.4480450
C	4.2609478	2.2403478	0.5604427
C	3.7479490	3.5216133	0.8248935
C	0.0035033	2.8733651	0.9142157
Pd	-2.4568268	4.6343843	-0.7525451
P	-2.1198246	6.8225822	0.0788907
C	-0.9036536	2.2889368	0.0636635
Br	-1.9375400	5.3425062	-3.0976223
C	-0.5171954	1.4314938	-1.0926075
C	0.2456565	1.9816869	-2.1444664
C	0.5798561	1.2027656	-3.2604032

C	0.1549101	-0.1341714	-3.3424354
C	-0.6204349	-0.6847709	-2.3084960
C	-0.9626781	0.0971665	-1.1939402
C	-0.4632922	3.9366352	1.9042690
O	0.3441183	4.0197760	3.0745673
C	-1.9391801	3.7962312	2.2743627
C	-2.8607917	3.5322687	1.1027136
C	-2.3504957	2.6312811	0.1145416
C	-4.3391516	3.5461396	1.4170953
H	-0.3286525	4.9209244	1.4022730
H	-2.2530935	4.6815988	2.8555063
H	-2.0369170	2.9221677	2.9650974
H	-3.0295007	1.8836077	-0.3286292
H	-2.6372926	3.2858414	-1.5452974
H	-4.5746926	2.8070095	2.2170785
H	-4.9547076	3.3038116	0.5288892
H	-4.6501978	4.5389777	1.7971157
H	0.4841422	3.1080950	3.3942693
H	1.3154672	0.4907373	0.4941061
H	3.7677423	0.1419262	0.2568281
H	5.3456231	2.0879653	0.4530342
H	4.4295322	4.3800828	0.9263169
H	1.9844172	4.7219013	1.1840019
H	-1.5658778	-0.3359518	-0.3802952
H	-0.9618200	-1.7293859	-2.3701406
H	0.4193657	-0.7451163	-4.2187970
H	1.1680008	1.6474719	-4.0770318
H	0.5586372	3.0336923	-2.0849451
C	-3.2391282	8.1583646	-0.5172285
C	-0.4154110	7.3761486	-0.3415604
C	-2.1863795	7.0469824	1.9023357
C	-1.0181028	7.1051277	2.6870496
C	-1.1065154	7.0902294	4.0886230
C	-2.3601282	7.0426002	4.7171396
C	-3.5323058	7.0112494	3.9391974
C	-3.4471973	7.0032102	2.5403906
H	-0.0324452	7.1456397	2.2024168
H	-0.1849746	7.1067892	4.6883867
H	-2.4273789	7.0308972	5.8153889
H	-4.5186572	6.9818848	4.4264867
H	-4.3648196	6.9682526	1.9327836
C	-3.4410624	9.3333140	0.2411791
C	-4.2748043	10.3516872	-0.2452732
C	-4.9156457	10.2048309	-1.4871275
C	-4.7200014	9.0356618	-2.2403350
C	-3.8869625	8.0125951	-1.7610308

H	-2.9568404	9.4463786	1.2225137
H	-4.4266528	11.2635704	0.3521569
H	-5.5715662	11.0034900	-1.8660440
H	-5.2200995	8.9138011	-3.2130336
H	-3.7126575	7.1033947	-2.3581389
C	0.5361360	6.4054522	-0.7149730
C	1.8658467	6.7784594	-0.9638248
C	2.2486404	8.1253024	-0.8568989
C	1.2988126	9.0992236	-0.5017315
C	-0.0293832	8.7277741	-0.2431740
H	0.2211406	5.3571023	-0.8287152
H	2.5993280	6.0101709	-1.2502384
H	3.2893499	8.4204892	-1.0599459
H	1.5932773	10.1571470	-0.4288150
H	-0.7701574	9.4942262	0.0286519

S4

75

SCF Energy = -4548.336085906

C	-1.1117721	2.8775316	-2.5189159
C	-0.6785729	2.0274512	-1.4761768
C	-0.1597357	0.7564784	-1.8129399
C	-0.0647904	0.3534606	-3.1510096
C	-0.4865113	1.2125122	-4.1807906
C	-1.0105609	2.4750364	-3.8592658
C	-0.7806642	2.4494192	-0.0532967
C	0.2594554	2.3525560	0.8364863
C	1.6387548	1.9784046	0.4423965
C	2.3700324	1.0270384	1.1885973
C	3.6776656	0.6758635	0.8214698
C	4.2849199	1.2845831	-0.2891775
C	3.5756585	2.2481594	-1.0273407
C	2.2661692	2.5903805	-0.6673879
Br	-1.5932215	7.2384900	-0.3251482
C	-2.4127182	3.1739726	1.7670826
C	-3.8536502	3.0570022	2.2154232
C	-2.0972228	2.9939331	0.3792190
C	-1.3653369	2.7023883	2.7529370
C	0.0739384	2.8649179	2.2578764
O	0.5435467	4.2208384	2.3133124
H	0.7481085	2.3133413	2.9433076
H	-1.4798876	3.1993555	3.7350874
H	-1.5459760	1.6146270	2.9281325
H	-2.9321369	2.7804731	-0.3084260
H	-2.0600857	4.5609079	-0.5237440
H	-4.0225715	3.6033899	3.1620398

H	-4.1091414	1.9901834	2.4083476
H	-4.5583477	3.4462958	1.4552334
H	0.0001455	4.7253629	1.6501537
H	1.8977136	0.5380607	2.0549993
H	4.2258561	-0.0783382	1.4065022
H	5.3125144	1.0136707	-0.5753825
H	4.0492810	2.7414614	-1.8896338
H	1.7149018	3.3492134	-1.2406517
H	0.1703840	0.0842622	-1.0077903
H	0.3402188	-0.6409687	-3.3929254
H	-0.4082509	0.8969163	-5.2322217
H	-1.3376874	3.1583861	-4.6575464
H	-1.4966386	3.8817745	-2.2806332
Pd	-2.0285916	5.1436760	0.9369278
P	-2.1178227	6.3992017	2.9523821
C	-0.8428162	7.7228467	3.0433695
C	0.5199507	7.3730910	2.9192594
H	0.8182858	6.3226758	2.7899077
C	1.5061789	8.3693546	2.9476809
H	2.5645929	8.0839180	2.8518742
C	1.1462558	9.7209692	3.0752594
H	1.9221392	10.5014581	3.0845961
C	-0.2087818	10.0726084	3.1728747
H	-0.5018296	11.1303806	3.2535142
C	-1.2013554	9.0803419	3.1554897
H	-2.2596172	9.3694574	3.2105501
C	-2.0222247	5.5311255	4.5761905
C	-0.7790058	5.2729336	5.1902495
H	0.1431914	5.6840256	4.7606115
C	-0.7104701	4.4784868	6.3447446
H	0.2673460	4.2885195	6.8125250
C	-1.8770546	3.9258683	6.8988133
H	-1.8188050	3.2996966	7.8018256
C	-3.1194946	4.1842800	6.2972855
H	-4.0416552	3.7657389	6.7282526
C	-3.1932382	4.9820448	5.1450492
H	-4.1729622	5.1920101	4.6920042
C	-3.7279528	7.2752437	3.0628611
C	-4.1299798	7.9193236	4.2543815
H	-3.4785299	7.8895962	5.1407745
C	-5.3590832	8.5918593	4.3102453
H	-5.6661124	9.0925913	5.2409805
C	-6.1951550	8.6270741	3.1799056
H	-7.1600164	9.1547317	3.2262908
C	-5.7976368	7.9906808	1.9933875
H	-6.4461636	8.0199639	1.1050151

C	-4.5672014	7.3166502	1.9319764
H	-4.2365621	6.8338180	0.9990671

Optimized Geometries(BXnl)

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R4
75
SCF Energy = -4548.331865813
C      1.3415718   -2.8039462    2.5036629
C      0.2389730   -3.2765960    1.7482454
C      0.1241290   -4.6726890    1.5434194
C      1.0915756   -5.5569432    2.0382788
C      2.1977127   -5.0695789    2.7547007
C      2.3137350   -3.6888193    2.9883312
C     -0.7457005   -2.3209398    1.1916407
Pd     -0.8396410    0.1963563   -1.1818885
P      0.0919587    1.9661414    0.1556793
C     -1.2785627   -2.4396208   -0.0712489
Br     1.0560109    0.4126074   -2.7818304
C     -0.8594974   -3.4849822   -1.0479671
C      0.4749136   -3.5204732   -1.5050591
C      0.8742585   -4.4695943   -2.4552883
C     -0.0535450   -5.3943718   -2.9642972
C     -1.3883112   -5.3549203   -2.5285405
C     -1.7909368   -4.3991162   -1.5822550
C     -1.0421438   -1.0746678    2.0201919
O     -1.0085492   -1.3037429    3.4259803
C     -2.3451993   -0.3807261    1.6219399
C     -2.5948796   -0.2864500    0.1323894
C     -2.1923705   -1.4133497   -0.6263966
C     -3.7839926    0.5436596   -0.2877661
H     -0.2049108   -0.3650920    1.8376710
H     -2.3988325    0.6033723    2.1197565
H     -3.1905170   -0.9820113    2.0398626
H     -2.7839129   -1.7186216   -1.5030311
H     -1.1737012   -0.7808760   -2.3484039
H     -4.7088081    0.1754618    0.2126860
H     -3.9443471    0.5138970   -1.3828570
H     -3.6555823    1.6006457    0.0184307
H     -1.5244917   -2.1145530    3.5976255
H     -0.7392522   -5.0656440    0.9900884
H      0.9790151   -6.6376220    1.8629054
H      2.9599957   -5.7639713    3.1394036

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H	3.1686847	-3.2942381	3.5585783
H	1.4421471	-1.7300965	2.7055363
H	-2.8363102	-4.3713434	-1.2362885
H	-2.1214731	-6.0719925	-2.9283774
H	0.2617401	-6.1399473	-3.7098919
H	1.9161886	-4.4797964	-2.8087425
H	1.1926294	-2.7828940	-1.1189632
C	0.1947817	3.6226232	-0.6481715
C	1.8126676	1.5098713	0.6256334
C	-0.6688892	2.4023362	1.7731858
C	-0.1458100	1.9313798	2.9933308
C	-0.8528087	2.1315310	4.1901235
C	-2.0723639	2.8253876	4.1828294
C	-2.5859475	3.3248749	2.9717599
C	-1.8943578	3.1074490	1.7725231
H	0.8125249	1.3930559	3.0084183
H	-0.4461882	1.7335400	5.1311173
H	-2.6249002	2.9812177	5.1215681
H	-3.5371312	3.8784188	2.9610237
H	-2.3018404	3.4919118	0.8246280
C	0.3683856	4.7916922	0.1270290
C	0.4578209	6.0457436	-0.4952406
C	0.3659337	6.1465151	-1.8938302
C	0.1825663	4.9883948	-2.6662165
C	0.0960333	3.7298715	-2.0501376
H	0.4138894	4.7235938	1.2241222
H	0.5945730	6.9496733	0.1177084
H	0.4325138	7.1314356	-2.3807573
H	0.1055530	5.0599647	-3.7616591
H	-0.0238284	2.8187961	-2.6554212
C	2.1691186	0.1460358	0.5986692
C	3.4410746	-0.2620761	1.0272274
C	4.3720862	0.6924855	1.4678254
C	4.0278276	2.0554164	1.4788175
C	2.7519909	2.4648090	1.0615377
H	1.4472985	-0.5937007	0.2202032
H	3.7022740	-1.3305078	1.0069820
H	5.3738183	0.3754906	1.7956673
H	4.7594823	2.8070531	1.8119847
H	2.4913139	3.5331454	1.0664645

S4

75

SCF Energy = -4548.336784080

C	-0.7097712	-3.7389564	-2.5070128
C	-1.0300436	-3.9300590	-1.1439057

C	-1.3764335	-5.2307148	-0.7103671
C	-1.3837584	-6.3069771	-1.6063721
C	-1.0458835	-6.1073072	-2.9564255
C	-0.7106474	-4.8188872	-3.4027472
C	-1.0331980	-2.7892957	-0.1889876
C	-0.4582535	-2.8506090	1.0578446
C	0.4006878	-3.9695053	1.5117509
C	0.2330058	-4.5381237	2.7945634
C	1.0515322	-5.5920578	3.2272635
C	2.0660006	-6.0855755	2.3906076
C	2.2572272	-5.5145226	1.1201574
C	1.4334716	-4.4692646	0.6845093
Br	1.5800759	0.8390218	-2.3534225
C	-2.0640415	-0.5145769	0.2648553
C	-3.2425498	0.3846423	-0.0339960
C	-1.7224208	-1.5539647	-0.6384211
C	-1.7518052	-0.7729161	1.7218147
C	-0.4948941	-1.6179536	1.9484227
O	0.7250409	-0.8822837	1.7597364
H	-0.4657870	-1.9256097	3.0129187
H	-1.6831002	0.1654263	2.3024102
H	-2.6200803	-1.3371616	2.1388434
H	-2.3094097	-1.6512044	-1.5649502
H	-0.2665948	-0.9367041	-2.0768539
H	-3.1235919	1.3799095	0.4325736
H	-4.1720942	-0.0593309	0.3886825
H	-3.3919078	0.5228497	-1.1220948
H	0.7832934	-0.6913978	0.7860873
H	-0.5671393	-4.1648102	3.4527359
H	0.8953949	-6.0313652	4.2244020
H	2.7116827	-6.9094743	2.7304971
H	3.0598782	-5.8841845	0.4641087
H	1.5886623	-4.0178423	-0.3057908
H	-1.6440688	-5.3886196	0.3442009
H	-1.6585592	-7.3110010	-1.2488133
H	-1.0481785	-6.9541582	-3.6593568
H	-0.4413114	-4.6507122	-4.4565465
H	-0.4233058	-2.7363008	-2.8605468
Pd	-0.3151146	0.1267534	-0.9400470
P	0.0067704	2.1571537	0.3496219
C	1.7896788	2.5612955	0.5717131
C	2.6213369	1.6370659	1.2419617
H	2.2061289	0.6991297	1.6383490
C	3.9903661	1.9016552	1.3896740
H	4.6270273	1.1742458	1.9155196
C	4.5490111	3.0729172	0.8525760

H	5.6260607	3.2720269	0.9600447
C	3.7297443	3.9787564	0.1615656
H	4.1616843	4.8885659	-0.2822288
C	2.3566734	3.7256758	0.0181095
H	1.7314458	4.4298765	-0.5470934
C	-0.7344256	2.4305330	2.0195856
C	-0.0687695	1.9978172	3.1861251
H	0.9443206	1.5823769	3.1194830
C	-0.7008254	2.0790556	4.4357518
H	-0.1652324	1.7389923	5.3349532
C	-2.0070155	2.5855414	4.5415039
H	-2.5017128	2.6428246	5.5227811
C	-2.6737301	3.0260419	3.3870432
H	-3.6927331	3.4358424	3.4576010
C	-2.0424962	2.9523020	2.1356127
H	-2.5689024	3.3184881	1.2425811
C	-0.6915800	3.5586877	-0.6115753
C	-0.7439849	4.8641549	-0.0732677
H	-0.3653727	5.0539973	0.9423859
C	-1.2834010	5.9158896	-0.8274377
H	-1.3192407	6.9305111	-0.4025666
C	-1.7768705	5.6742209	-2.1221521
H	-2.2009174	6.5011132	-2.7119910
C	-1.7276498	4.3788467	-2.6607091
H	-2.1095186	4.1852005	-3.6742518
C	-1.1855973	3.3233431	-1.9096789
H	-1.1257766	2.3074897	-2.3310208

Optimized Geometries(MXn-TS-c-d-6)

R4
75
SCF Energy = -4548.304372085

C	1.7758721	4.3543837	-2.9994389
C	1.5881341	4.5724870	-1.6093069
C	1.0396319	5.8176836	-1.2174093
C	0.6496595	6.7761604	-2.1640143
C	0.8260250	6.5335182	-3.5345634
C	1.4055772	5.3192309	-3.9428926
C	1.9833210	3.5396008	-0.6187331
C	1.8418028	2.1721128	-0.8037652
C	1.0683815	1.6009867	-1.9306712
C	-0.2074649	2.1259464	-2.2549393

C	-0.9469430	1.6131446	-3.3275987
C	-0.4291350	0.5617149	-4.1039325
C	0.8260957	0.0168539	-3.7842199
C	1.5646096	0.5225977	-2.7052600
Br	5.4084591	4.0710603	2.3831917
C	2.1086735	3.0717435	2.0343395
C	2.3486858	3.4279577	3.4808483
C	1.3890949	3.9912864	1.1788021
C	1.9580116	1.6059805	1.7014138
C	2.3887578	1.1984881	0.2522760
O	2.0572313	-0.1605036	0.0184807
H	3.4984043	1.2255901	0.2308268
H	2.5427760	0.9864486	2.4093973
H	0.8923726	1.2967752	1.8074604
H	0.3721235	3.7555241	0.8216407
H	1.4517807	5.0493358	1.4933330
H	3.2349096	2.9047239	3.8874457
H	1.4594784	3.1286399	4.0834089
H	2.5099981	4.5141558	3.6181786
H	1.1057711	-0.1998324	-0.2012784
H	-0.6131429	2.9554541	-1.6576161
H	-1.9346600	2.0385327	-3.5614205
H	-1.0064091	0.1626970	-4.9516527
H	1.2353434	-0.8118082	-4.3821720
H	2.5375347	0.0838209	-2.4487669
H	0.9178020	6.0524735	-0.1534330
H	0.2201596	7.7289626	-1.8201503
H	0.5271917	7.2875196	-4.2782813
H	1.5738993	5.1144582	-5.0106850
H	2.2186990	3.4137235	-3.3437452
Pd	3.6138250	3.9156302	0.6621804
P	5.0635113	4.7420980	-0.9574461
C	4.8074360	6.5494103	-1.0172418
C	5.3638245	7.3117610	0.0371228
H	5.9900511	6.8163126	0.7956081
C	5.0926752	8.6830949	0.1282756
H	5.5317177	9.2696001	0.9494905
C	4.2558861	9.3051195	-0.8167008
H	4.0444485	10.3826530	-0.7417361
C	3.6810576	8.5437380	-1.8455307
H	3.0071729	9.0143824	-2.5770765
C	3.9476096	7.1686556	-1.9455574
H	3.4669744	6.5805745	-2.7382509
C	6.8793896	4.5172207	-0.7645125
C	7.3532418	3.2894091	-0.2614192
H	6.6378746	2.5432924	0.1128254

C	8.7313763	3.0359411	-0.2167889
H	9.0957244	2.0779544	0.1835685
C	9.6432609	4.0084359	-0.6616101
H	10.7252071	3.8116839	-0.6151060
C	9.1724562	5.2331589	-1.1622735
H	9.8825856	5.9978117	-1.5123209
C	7.7926592	5.4870047	-1.2209455
H	7.4266193	6.4453392	-1.6183041
C	4.8809290	4.0542167	-2.6523552
C	4.6017385	2.6744689	-2.7415328
H	4.4480983	2.0942567	-1.8200596
C	4.4993554	2.0531276	-3.9946952
H	4.2731467	0.9790383	-4.0558385
C	4.6679786	2.8065329	-5.1682707
H	4.5706989	2.3233272	-6.1521396
C	4.9758412	4.1751027	-5.0826150
H	5.1292140	4.7645426	-5.9993644
C	5.0972615	4.7954892	-3.8300364
H	5.3576866	5.8616967	-3.7716355

S4

75

SCF Energy = -4548.317001003

C	1.6481853	3.7627017	-3.1468911
C	0.9704067	4.1433655	-1.9588460
C	-0.2141100	4.9054829	-2.1030814
C	-0.7280492	5.2263368	-3.3678614
C	-0.0550624	4.8221384	-4.5305663
C	1.1452985	4.1001503	-4.4085043
C	1.5031114	3.7719532	-0.6254954
C	2.1131239	2.5739753	-0.3006455
C	2.2216283	1.4228829	-1.2233840
C	1.1240261	0.9923539	-2.0075602
C	1.2433996	-0.1114108	-2.8608430
C	2.4611925	-0.8087365	-2.9535048
C	3.5536102	-0.4040161	-2.1679780
C	3.4331731	0.6934350	-1.3038881
Br	3.1885198	6.8378871	2.3549259
C	1.0665433	4.1231919	2.0364516
C	0.6846534	4.8842512	3.2813824
C	0.2605730	4.2462102	0.8436516
C	1.7399245	2.7779744	2.2358786
C	2.7070700	2.3542186	1.0963614
O	3.9987625	2.9541292	1.2493749
H	2.8948534	1.2690839	1.2113756
H	2.3219406	2.7794936	3.1788912

H	0.9608704	1.9869165	2.3363023
H	-0.3395290	3.3981326	0.4742421
H	-0.2993800	5.1956612	0.7558488
H	1.5606877	5.0547670	3.9356208
H	-0.0663864	4.2900822	3.8525312
H	0.2418201	5.8710920	3.0478879
H	3.8369939	3.9358023	1.2328742
H	0.1691458	1.5330780	-1.9401335
H	0.3769564	-0.4335660	-3.4582763
H	2.5547597	-1.6716851	-3.6299719
H	4.5082420	-0.9488607	-2.2279374
H	4.2899325	1.0145609	-0.6923445
H	-0.7476132	5.2617354	-1.2137886
H	-1.6556665	5.8135303	-3.4394683
H	-0.4535120	5.0784622	-5.5237730
H	1.7028432	3.7916683	-5.3053706
H	2.5810798	3.1936819	-3.0787958
Pd	2.2698270	5.3074380	0.6205354
P	3.5310181	6.3898803	-1.0230424
C	5.0511425	7.3116996	-0.5501397
C	5.9371654	6.7132817	0.3678311
H	5.6602271	5.7711923	0.8616333
C	7.1613949	7.3280703	0.6633226
H	7.8452767	6.8580034	1.3857564
C	7.5045991	8.5473571	0.0541412
H	8.4618405	9.0339885	0.2955841
C	6.6232439	9.1448790	-0.8609983
H	6.8876932	10.0988920	-1.3420940
C	5.4004040	8.5269179	-1.1692865
H	4.7149046	8.9956189	-1.8905842
C	4.2372708	5.3417969	-2.3557496
C	4.4248605	5.7929548	-3.6772226
H	4.1121709	6.8066085	-3.9654751
C	5.0093324	4.9464852	-4.6309293
H	5.1371370	5.2980143	-5.6660894
C	5.4376980	3.6585860	-4.2651608
H	5.8924588	2.9949335	-5.0161187
C	5.2970671	3.2260610	-2.9363376
H	5.6397067	2.2238443	-2.6417990
C	4.6966633	4.0611739	-1.9817094
H	4.5645533	3.7068063	-0.9476703
C	2.4205191	7.6417056	-1.7561528
C	2.1349752	8.7803274	-0.9648735
H	2.6414190	8.9104156	0.0046105
C	1.1923533	9.7192021	-1.4032437
H	0.9790003	10.6036634	-0.7841388

C	0.5148232	9.5281601	-2.6218374
H	-0.2254626	10.2675957	-2.9633085
C	0.7763664	8.3849573	-3.3919119
H	0.2360103	8.2133633	-4.3349040
C	1.7205982	7.4387539	-2.9612311
H	1.8918228	6.5337805	-3.5587553

Optimized Geometries(MXnd-6)

R4
75
SCF Energy = -4548.351903722

C	-2.4354944	0.7332127	-1.5687035
C	-2.1123379	1.7640846	-0.6558335
C	-2.1030863	3.0924027	-1.1466692
C	-2.3889639	3.3721421	-2.4915048
C	-2.6826579	2.3304531	-3.3861609
C	-2.7082834	1.0068776	-2.9125659
C	-1.7534225	1.5037977	0.7600239
C	-2.1655148	0.3790096	1.5436744
C	-3.0192761	-0.7370731	1.0385623
C	-4.3356571	-0.4973586	0.5930631
C	-5.1471489	-1.5616234	0.1745691
C	-4.6613834	-2.8801232	0.2110796
C	-3.3635532	-3.1307244	0.6873194
C	-2.5497068	-2.0653715	1.1037158
Br	1.8216503	-0.8565876	2.4892988
C	-0.2283069	1.8304029	2.5686830
C	1.0815586	2.4662953	2.9640641
C	-1.0671552	2.6159444	1.5603145
C	-1.0866697	1.2830907	3.6864455
C	-2.3014044	0.5448960	3.0792906
O	-3.5651536	1.1528232	3.3543194
H	-2.3801088	-0.4685240	3.5165159
H	-0.4906263	0.5949128	4.3181433
H	-1.4525062	2.1041224	4.3491370
H	-1.7738067	3.3457431	2.0358841
H	-0.4072500	3.1998678	0.8897627
H	1.6735561	1.8008024	3.6193070
H	0.8783288	3.4182878	3.5107875
H	1.6962774	2.7160298	2.0754559
H	-3.5366590	2.0495123	2.9679143
H	-4.7135530	0.5342923	0.5645973

H	-6.1689202	-1.3602945	-0.1813110
H	-5.2998016	-3.7133216	-0.1196880
H	-2.9802436	-4.1614072	0.7345221
H	-1.5274624	-2.2466576	1.4720710
H	-1.8630371	3.9244486	-0.4710631
H	-2.3726449	4.4150059	-2.8432627
H	-2.8888746	2.5473956	-4.4449971
H	-2.9181775	0.1704866	-3.5956424
H	-2.4380019	-0.3051712	-1.2309043
Pd	-0.0301620	0.2188018	1.2158893
P	0.6796090	-0.8570141	-0.8634973
C	1.5149440	0.7365513	-1.2540251
C	2.6998380	1.0651779	-0.5525637
H	3.1770892	0.3126636	0.0931178
C	3.2343969	2.3582675	-0.6394642
H	4.1539760	2.6014388	-0.0860671
C	2.5937421	3.3406245	-1.4150602
H	3.0114987	4.3571675	-1.4743751
C	1.4170792	3.0193582	-2.1114862
H	0.9024387	3.7799168	-2.7174906
C	0.8769858	1.7267410	-2.0339231
H	-0.0549456	1.4978260	-2.5677074
C	2.0159660	-2.1180560	-0.8410047
C	1.8617199	-3.2297190	0.0099586
H	1.0034101	-3.2718234	0.6958455
C	2.8141584	-4.2597646	-0.0016310
H	2.6919328	-5.1235715	0.6689309
C	3.9309236	-4.1765137	-0.8495418
H	4.6833569	-4.9798201	-0.8497725
C	4.0913228	-3.0639965	-1.6934583
H	4.9668489	-2.9951701	-2.3569630
C	3.1338073	-2.0383629	-1.6945922
H	3.2594016	-1.1681952	-2.3564552
C	-0.1897268	-1.3637814	-2.4106510
C	-1.2875790	-2.2388791	-2.2817967
H	-1.6232666	-2.5489603	-1.2809564
C	-1.9728672	-2.6897847	-3.4193978
H	-2.8366307	-3.3614365	-3.3024855
C	-1.5631018	-2.2742180	-4.6980155
H	-2.1043470	-2.6204093	-5.5915839
C	-0.4564471	-1.4183357	-4.8323374
H	-0.1250944	-1.0979212	-5.8318701
C	0.2325207	-0.9683158	-3.6954708
H	1.0984393	-0.3003395	-3.8101116

S4

75

SCF Energy = -4548.357056489

C	-0.6760211	-2.5840460	-1.4438257
C	-1.7585812	-2.2618846	-0.5919644
C	-3.0650479	-2.3622415	-1.1296214
C	-3.2762530	-2.7476877	-2.4622819
C	-2.1854016	-3.0361196	-3.2979434
C	-0.8825336	-2.9563640	-2.7759706
C	-1.5822626	-1.7640924	0.7976967
C	-0.4892779	-2.0854509	1.6644054
C	0.6056264	-3.0090839	1.2423942
C	0.3083799	-4.3544530	0.9417627
C	1.3265619	-5.2409395	0.5610922
C	2.6570495	-4.7956779	0.4869403
C	2.9642990	-3.4635800	0.8122841
C	1.9460947	-2.5766405	1.1935222
Br	0.8551799	1.6862074	2.5971669
C	-2.0272299	-0.0791284	2.4125047
C	-2.6488426	1.2745673	2.6421077
C	-2.7432195	-0.9941128	1.4288698
C	-1.5956719	-0.8661161	3.6297117
C	-0.5575507	-1.9332400	3.2128679
O	0.7172976	-1.6368661	3.7502749
H	-0.8158920	-2.9394834	3.6142163
H	-1.1235945	-0.2139235	4.3895040
H	-2.4905344	-1.3317523	4.1069627
H	-3.5131440	-1.6472632	1.9119900
H	-3.2550393	-0.3982009	0.6475300
H	-2.0094809	1.9070451	3.2861655
H	-3.6413454	1.1494879	3.1373900
H	-2.8227300	1.8062812	1.6846208
H	0.9170976	-0.7037742	3.4866336
H	-0.7363437	-4.6977415	0.9857417
H	1.0784274	-6.2848626	0.3165118
H	3.4560202	-5.4897245	0.1848278
H	4.0066134	-3.1117041	0.7722907
H	2.1737452	-1.5297340	1.4371459
H	-3.9346703	-2.1299708	-0.4998434
H	-4.3039171	-2.8145126	-2.8510456
H	-2.3480763	-3.3195181	-4.3486661
H	-0.0103885	-3.1609653	-3.4142528
H	0.3474408	-2.5030995	-1.0698956
Pd	-0.3264520	0.0191253	1.1390584
P	0.8727472	0.5985884	-0.8870906
C	2.1374377	1.9290473	-0.8758477
C	3.1853873	1.8422934	0.0610016

H	3.1788562	1.0360462	0.8082268
C	4.2117251	2.8000748	0.0548396
H	5.0253912	2.7317457	0.7923049
C	4.1876552	3.8516573	-0.8751869
H	4.9878853	4.6073667	-0.8726112
C	3.1387777	3.9436793	-1.8075509
H	3.1181717	4.7679532	-2.5366593
C	2.1178878	2.9822224	-1.8129239
H	1.2990421	3.0517355	-2.5450687
C	1.3614628	-0.3083456	-2.4143650
C	0.9096394	0.0444607	-3.7012973
H	0.2028567	0.8773154	-3.8287817
C	1.3525581	-0.6730403	-4.8233316
H	0.9891380	-0.3961986	-5.8246757
C	2.2550496	-1.7392966	-4.6715299
H	2.5962494	-2.3028783	-5.5530636
C	2.7210299	-2.0833658	-3.3906298
H	3.4264030	-2.9179901	-3.2615430
C	2.2774507	-1.3706543	-2.2674127
H	2.6252105	-1.6564592	-1.2631871
C	-0.7205758	1.4344503	-1.2748909
C	-1.0109585	2.6714106	-0.6500622
H	-0.2261110	3.1927029	-0.0820355
C	-2.3048391	3.2085710	-0.7194565
H	-2.5192114	4.1685418	-0.2262646
C	-3.3236928	2.5192690	-1.3993834
H	-4.3398598	2.9395143	-1.4434540
C	-3.0407790	1.2905052	-2.0208676
H	-3.8310840	0.7392837	-2.5520346
C	-1.7493066	0.7479100	-1.9628335
H	-1.5471815	-0.2233980	-2.4345287

Optimized Product Geometries(Xn)

R3
38
SCF Energy = -809.6157366451

C	-2.4394944	4.1865518	0.9217375
C	-1.1662954	3.7324715	0.4654712
C	-0.6563585	4.1756099	-0.7696322
C	-1.4150534	5.0748330	-1.5365083
C	-2.6650931	5.5326955	-1.0782907
C	-3.1833077	5.0889691	0.1537083

C	-0.6451582	2.8079675	1.4741914
C	0.5559398	2.3883967	1.9717624
C	1.9225189	2.6756043	1.5083326
C	2.9527327	1.7231771	1.7085824
C	4.2652644	1.9902063	1.2935146
C	4.5817079	3.2144218	0.6815261
C	3.5729138	4.1766721	0.4968498
C	2.2594108	3.9121587	0.9061204
C	-1.8330590	2.3292665	2.3200094
C	-2.5450604	1.1355227	1.6443513
C	-2.7726235	3.5700846	2.2718758
C	-1.1426006	1.9121366	3.6347923
C	0.3033351	1.5235582	3.2114075
O	0.4924857	0.1226418	2.9518626
H	1.0317150	1.7532799	4.0169917
H	-1.0879865	2.7805724	4.3232933
H	-1.6385552	1.0789711	4.1706716
H	-2.5097499	4.2824709	3.0853552
H	-3.8477859	3.3224188	2.3845720
H	-1.8742315	0.2567010	1.5688742
H	-2.8853926	1.3965679	0.6219707
H	-3.4302566	0.8288811	2.2383704
H	0.1199479	-0.0482385	2.0655012
H	2.6974328	0.7627387	2.1804755
H	5.0493854	1.2334808	1.4500373
H	5.6124679	3.4229388	0.3569654
H	3.8149764	5.1479970	0.0385795
H	1.4839315	4.6821741	0.7875324
H	0.3132335	3.8094897	-1.1360719
H	-1.0313830	5.4200484	-2.5085537
H	-3.2462214	6.2370503	-1.6928418
H	-4.1652329	5.4442117	0.5033124

R4

38

SCF Energy = -809.6147734832

C	4.4336826	1.3998109	-0.0605547
C	3.0374005	1.2285851	-0.2337869
C	2.5937668	0.4130502	-1.3039908
C	3.5062372	-0.1763945	-2.1882740
C	4.8874690	0.0278742	-2.0214756
C	5.3446183	0.8133970	-0.9502862
C	2.0885769	1.8478284	0.7019706
C	0.8102987	2.2794397	0.4944339
C	-0.2145794	2.2938567	-0.5497247
C	-0.1373923	2.2708299	-1.9559222

C	-1.3239419	2.3099946	-2.7056849
C	-2.5767463	2.3645942	-2.0657107
C	-2.6614427	2.3942588	-0.6604865
C	-1.4848611	2.3688064	0.0963905
C	2.4427699	2.0471756	2.1882649
O	3.2825988	1.0474176	2.7386002
C	1.0491238	2.1643487	2.8650876
C	0.1675630	2.8133528	1.7810874
C	-1.3191410	2.3943117	1.6079519
C	0.2656843	4.3554878	1.8261783
H	3.0139933	2.9945518	2.3251854
H	1.0813976	2.7171112	3.8250446
H	0.6948445	1.1316953	3.0738354
H	-1.4852801	1.3747638	2.0228421
H	-2.0364428	3.0743587	2.1109612
H	-0.2043428	4.7470534	2.7515935
H	-0.2530015	4.8078030	0.9568577
H	1.3203661	4.6950329	1.8027742
H	2.9257504	0.1858069	2.4472598
H	1.5174714	0.2238666	-1.4225164
H	3.1371196	-0.8094177	-3.0098766
H	5.6046931	-0.4342741	-2.7165946
H	6.4244429	0.9678859	-0.8024138
H	4.8042186	1.9942264	0.7855314
H	-3.6434257	2.4466164	-0.1648074
H	-3.4967947	2.3949599	-2.6691077
H	-1.2734062	2.3044664	-3.8051248
H	0.8390111	2.2417674	-2.4599121

S3

38

SCF Energy = -809.6138763928

C	-2.0096176	3.0633477	1.7080276
C	-1.1846378	3.1572011	0.5456128
C	-1.7074414	3.7238738	-0.6355935
C	-3.0407057	4.1619789	-0.6570113
C	-3.8566254	4.0428391	0.4835745
C	-3.3387756	3.4997106	1.6739449
C	0.1515277	2.6819129	0.9094138
C	1.4509350	2.8372164	0.5068563
C	1.9371178	3.2490907	-0.8193537
C	1.2267597	2.8479378	-1.9799133
C	1.6603594	3.2132507	-3.2609308
C	2.8284133	3.9789232	-3.4187700
C	3.5649004	4.3537984	-2.2827084
C	3.1315307	3.9917343	-0.9993508

C	0.0483559	1.9395687	2.2447278
C	-0.1611427	0.4329826	1.9685294
C	-1.2254884	2.5358123	2.8973209
C	1.4337278	2.2008080	2.8663536
C	2.3868441	2.4210315	1.6578110
O	3.4177431	3.3657970	1.9481737
H	2.9395357	1.4925273	1.3919973
H	1.4089884	3.1485853	3.4462670
H	1.7847581	1.4026698	3.5501528
H	-0.9666098	3.3809956	3.5738587
H	-1.7973401	1.8028568	3.5024996
H	0.6808742	0.0138476	1.3818804
H	-1.0926160	0.2632619	1.3912208
H	-0.2373040	-0.1297970	2.9219283
H	2.9628290	4.2044289	2.1634773
H	0.3432752	2.2036657	-1.8632831
H	1.0912983	2.8842231	-4.1440739
H	3.1713294	4.2674820	-4.4239894
H	4.4920262	4.9365340	-2.3962972
H	3.7206772	4.2650831	-0.1146288
H	-1.0803556	3.8253254	-1.5310911
H	-3.4531715	4.5977939	-1.5796606
H	-4.9037324	4.3799106	0.4453144
H	-3.9718426	3.4251902	2.5720131

S4

38

SCF Energy = -809.6157348489

C	-0.1932313	3.3724852	-1.5472439
C	-0.0491248	2.7802067	-0.2782736
C	-1.1882905	2.2616693	0.4063073
C	-2.4547787	2.3226776	-0.1851351
C	-2.5914755	2.9118880	-1.4569434
C	-1.4703276	3.4360686	-2.1280677
C	1.1123644	2.5754624	0.5892187
C	2.4575478	2.3621078	0.4846286
C	3.3291009	2.3948494	-0.7003167
C	4.6883110	2.7739176	-0.5690884
C	5.5382007	2.7889563	-1.6843324
C	5.0561583	2.4158587	-2.9499615
C	3.7149487	2.0166356	-3.0893804
C	2.8612616	2.0046778	-1.9786006
C	0.5912611	2.3636710	2.0172048
C	0.3472555	3.7173956	2.7218110
C	-0.7818285	1.6789695	1.7513791
C	1.7508652	1.5821916	2.6685004

C	3.0135279	2.0185301	1.8707021
O	3.7415697	3.1103689	2.4567817
H	3.7553264	1.1947385	1.8133390
H	1.8798887	1.7690824	3.7528157
H	1.5996704	0.4926995	2.5221784
H	-0.6501988	0.5778430	1.6596060
H	-1.5326357	1.8563765	2.5481945
H	1.2915077	4.2845041	2.8430398
H	-0.0752710	3.5536225	3.7342537
H	-0.3607169	4.3481605	2.1471377
H	3.2454358	3.9231117	2.2401297
H	5.0579315	3.0728338	0.4230399
H	6.5886128	3.0954735	-1.5632365
H	5.7246273	2.4271910	-3.8242197
H	3.3332377	1.7009600	-4.0726075
H	1.8230615	1.6609486	-2.0900056
H	-3.3365223	1.9215458	0.3385655
H	-3.5849733	2.9710287	-1.9269881
H	-1.5968549	3.9065036	-3.1149494
H	0.6782573	3.7946883	-2.0676832

PPh₃-Pd(H)Br

37
SCF Energy = -3738.694650155

Pd	0.9104044	-0.2993020	-4.3544411
P	-0.5485020	1.3477324	-4.7308459
C	-0.7234497	2.6137654	-3.4151195
C	-0.0026431	2.3031185	-6.1999752
C	-2.2653263	0.8349643	-5.1243907
C	-0.6561171	2.2060289	-2.0670507
C	-0.8346898	3.1447512	-1.0402705
C	-1.0695421	4.4948473	-1.3521249
C	-1.1248763	4.9066187	-2.6942568
C	-0.9526226	3.9708228	-3.7262788
H	-0.4475965	1.1517227	-1.8286156
H	-0.7781016	2.8215585	0.0099488
H	-1.2005062	5.2312755	-0.5449348
H	-1.2999453	5.9647419	-2.9409293
H	-0.9879787	4.2944854	-4.7774516
C	-0.8027458	2.4518571	-7.3497984
C	-0.3085045	3.1597223	-8.4577941
C	0.9798083	3.7174612	-8.4241855
C	1.7820323	3.5660575	-7.2788643

C	1.2974624	2.8572333	-6.1714425
H	-1.8115508	2.0146201	-7.3767478
H	-0.9365039	3.2746834	-9.3541461
H	1.3638592	4.2689374	-9.2955259
H	2.7938217	3.9974872	-7.2510106
H	1.9266776	2.7330509	-5.2753323
C	-3.3703441	1.6820503	-4.9051304
C	-4.6577420	1.2593180	-5.2712564
C	-4.8462880	-0.0041982	-5.8569830
C	-3.7460048	-0.8517120	-6.0715522
C	-2.4576397	-0.4375087	-5.7013674
H	-3.2244959	2.6687643	-4.4408361
H	-5.5199005	1.9198408	-5.0938895
H	-5.8576066	-0.3334174	-6.1398995
H	-3.8919497	-1.8455911	-6.5204943
H	-1.5891936	-1.1003128	-5.8466025
Br	2.5848508	-1.9987398	-4.0729183
H	-0.0956494	-0.7262353	-3.3055863

H₂CO₃

6
 SCF Energy = -264.8348300398

C	0.0402681	0.0000000	-0.0453569
O	-1.1650778	0.0000000	-0.6458897
O	-0.1071487	-0.0000000	1.3143124
O	1.0938675	-0.0000000	-0.6331674
H	-1.8564089	-0.0000000	0.0467565
H	0.7992238	0.0000000	1.6844012

HBr

2
 SCF Energy = -2574.735621963

H	0.0000000	0.0000000	-0.2138301
Br	0.0000000	0.0000000	1.2218301

HCO₃⁻

5
 SCF Energy = -264.2670446301

C	0.0416374	0.0000000	0.0725983
O	-0.1553027	-0.0000000	1.3176595
O	1.0735796	-0.0000000	-0.6222903
O	-1.2044528	-0.0000000	-0.7012735
H	-1.8435775	0.0000000	0.0386950

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