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Design and synthesis of phosphorus stabilised low valent group 14 elements

DISSERTATION

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The most effective way to do it, is to do it.

Amelia Earhart

AFFIDAVIT

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Abstract

In the last decades, organometallic chemistry and in particular heavier main-group elements got more and more attention. A vast number of transition metal complexes with phosphane ligands can be found in literature, but also in main group chemistry they are getting more prominent. Diphosphatetrylenes, the heavier analogues of the well known diaminotetrylenes, have gained interest in recent years. Those acyclic compounds have, due to their high reactivity, substantial possibilities in catalysis while still showing enough stability for convenient use. A comprehensive investigation of factors influencing the stabilisation of low valent diphospha main group compounds, such as the effective orbital overlap (π-type interaction) and the shielding of the active centre E (Ge, Sn), is still missing.

For this work the influence of various substituents (H, Me, ^{t}Bu, Ph, TMS, Hyp = ($Si(SiMe_3)_3$)) on the pyramidalisation of the phosphorus centres was studied by DFT analysis. For the stabilisation of tetrylenes various substituent combinations on P were evaluated. The steric bulk of phosphane ligands was determined with the exact cone angle method.[1] Through these considerations, ligand systems capable of isolating a stable E(II) (Ge, Sn) species were determined and used for the experimental approach.
The synthetic work led to the isolation of a number of novel phosphanes and phosphanides, characterised *via* NMR and single crystal X-ray crystallography. Those were further used for the synthesis of diphosphagermylenes and -stannylenes. Two novel monomeric diphosphastetrylenes were isolated and characterised by NMR. A Ge-P cubane, the first of this type, could be isolated characterised *via* NMR and single crystal X-ray diffractometry.
The knowledge gained in the synthesis of silylphosphanes was uses to examine and perform research on silylboranes, which are together with the investigated tetrylenes, auspicious candidates for catalysis and the activation of small molecules.

Danksagung

An dieser Stelle möchte ich mich bei all denjenigen bedanken, die mich während der Anfertigung meiner Doktorarbeit unterstützt und motiviert haben.
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Ein besonderer Dank geht auch an meine Studenten, danke für die gute Zusammenarbeit. Vielen Dank an meine Kollegen in Kassel mit denen ich einige Zeit im Labor und auf Konferenzen verbringen durfte.
Das Beste kommt bekanntlich zum Schluss, und ohne sie wäre ich vermutlich nicht so weit gekommen mit meinem Latein, ich bedanke mich bei meinen Freunden und ich bedanke mich bei meiner Familie.

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Eli Schwarz

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Contents

Index of abbreviations

B	Beckes B88 functional
B3	Beckes 3-parameter hybrid functional
CGTO	contracted Gauss-type orbitals
DFT	density functional theory
DZ	double zeta basis
ECP	effective core potential, pseudopotential
eV	electronvolt
GIAO	gauge invariant/independent atomic orbitals
GTF	Gauss-type function
HF	Hartree-Fock
HOMO	highest occupied molecular orbital
Hyp	tris(trimethylsilyl)silane
I	intensity
IR	infrared
K	Kelvin
KS	Kohn-Sham
LCAO	linear combination of atomic orbitals
LUMO	lowest unoccupied molecular orbital
LYP	Lee, Yang, Paar correlation functional
m-	meta
NHC	N-heterocyclic carbene
NMR	nuclear magnetic resonance
MO	molecular orbital
Ph	phenyl group
ppm	parts per million
SCF	self consistent field

STO	slater-type orbital
TZ	triple zeta basis
UV	ultraviolet
VIS	visible
ZPE	zero point vibrational energy
E	Energy
$\widehat{H}$	Hamilton operator
Ψ	total wave function of the system
r	space coordinates
ρ	electron density

Chapter 1

Introduction

1.1. Ligands in organometallic chemistry

Organometallic compounds are widely used both in research and industrial chemical reactions, where they predominantly act as catalysts, increasing reaction rates.[2]

Common examples are all Grignard reagents, metallocene compounds (ferrocene complexes), transition metal complexes and organolithium reagents. The latter ones are, together with organomagnesium- and aluminium reagents, widely used in homogeneous catalysis and commercial reactions.[2] The performance of a catalyst is dependent on the electronic and steric environment of the metal-ligand bond. Therefore specific designing is preferable. A ligand should be convenient to prepare in decent amounts and from easily accessible educts. Additionally, their structures should be stable and simple, and give the possibility of various uses.

1.1.1. Phosphanes

With the rapidly growing organometallic chemistry, began the search for ligands which could stabilise various metal oxidation states and could coordinate to diverse metals. The phosphane coordination chemistry startet with

the work of Hoffman[3] who reported the first complexes of triethylphosphane, trimethylphosphane, platinum and gold.[4] Subsequently, the ligand effect and coordination of phosphanes (former phosphines) was greatly acknowledged. Electron-rich, sterically demanding ligands were favoured, two examples are tri(t-butyl)phosphane and tri(cyclohexyl)phospane.[5]
In general, phosphanes turned out to be tremendous ligands in homogenous catalysis and were therefore a key factor in the development of organometallic chemistry.[4]
Phosphanes have the general formula PR_3 where R = alkyl, aryl, silyl, H or a halide. Closely related are phosphite ligands which have the general formula $P(OR)_3$. Organic phosphane derivatives arise through the formal exchange of hydrogen H for organic groups R. Depending on the degree of substitution, a distinction in monophosphanes, primary organo phosphanes, secondary and tertiary phosphanes, is made (see fig.1.1).

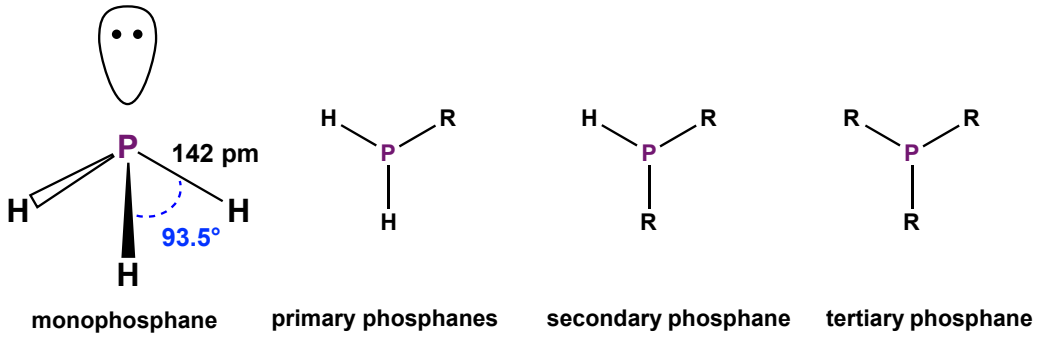


Figure 1.1.: Nomenclature of phosphanes

Primary phosphanes, like the simplest primary phosphane, methylphosphane, are synthesised *via* alkylation with alkali metal derivatives (M = Li, Na, K) see fig.1.2 or treating chlorophosphanes with hydrides.[6]

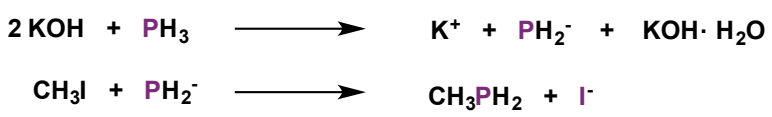


Figure 1.2.: Deprotonation-methylation procedure for methylphosphane[7]

Analogous to primary phosphanes, secondary phosphanes can be prepared by alkali-metal cleavage of triarylphosphanes, followed by the hydrolysis of the phosphide salt (e.g. synthesis of diphenylphosphane[8] fig.1.3).

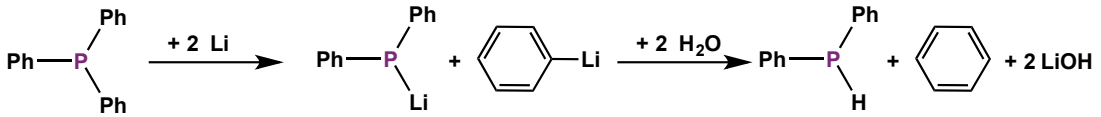


Figure 1.3.: Reaction of triphenylphosphane and lithium metal in tetrahydrofuran, studied by Wittenberg and Gilman[8]

A reaction of phosphorus trichloride or triphenylphosphite with organolithium reagents or Grignard reagents leads to tertiary phosphanes. Primary and secondary phosphanes are much less readily available than tertiary phosphanes. The primary species are highly toxic, spontaneously flammable gases or low-boiling liquids, which makes working under ambient conditions challenging.[9] Yet these phosphanes are of interest, as their functionalities can be changed rather easily. They can provide the necessary environment for a complex (activity or selectivity in homogeneous catalysis, reversible binding of a ligand, facile decomposition, or high stability).[10]

Still, research on transition metal complexes of primary and secondary phosphanes is much less developed than of tertiary phosphane complexes.[6] Similar to NH_3, phosphanes have a lone pair on the central atom that can be donated to a metal. Unlike NH_3, they are also π acids, to an extent that depends on the nature of the R groups present on the PR_3 ligand. For alkyl phosphanes, the π acidity is weak; aryl, dialkylamino, and alkoxy groups are successively more effective in promoting π acidity. In the extreme case of PF_3, the π acidity becomes quite similar to CO (widely used as ligand in organometallic chemistry). There are two general ways of bonding in phosphane ligands, similar to carbonyls:

The primary part is sigma donation of the phosphane lone pair to an empty orbital on the metal. The second way is the backdonation from a filled metal orbital to an empty orbital on the phosphane ligand. The empty orbital on the phosphorus can either be a d-orbitals or an antibonding sigma orbital. However, because of the high energy of the phosphorus d-orbital, donation into σ^* is more likely to happen.[11] As seen in fig.1.4 the σ^* orbitals of the P-R bonds are acting as acceptors in metal complexes, a more electronegative group in-

creases the stability of the P-R bond. As a result of an electronegative R (= N, O, F) the distribution of the P lone pair into the σ* orbital increases and with that also the overlap of the σ* with the metal centre M increases, giving higher stability.[10] The π acidity increases as follows: $PMe_3 \sim P(NR_2)_3 < PAr_3 < P(OMe)_3 < P(OAr)_3 < PCl_3 < CO \sim PF_3$.[10]

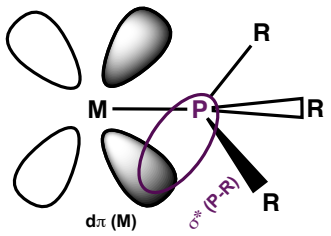


Figure 1.4.: Backdonating of the σ* in metal complexes of PR_3[10]

Even stronger complexes can be gained by covalent bonding with phosphanides. Therefore the metallation of PH_2 groups in phosphanes for further functionalisation was a great accomplishment. The direct metallation of primary or secondary phosphanes with a strong deprotonating agent such as an alkyllithium or an alkali metal hydride is the most common method. For that, highly-pure, conveniently soluble and accessible phosphanides were required. The very high sensitivity to air and moisture presents considerable disabilities and requires special working methods.[12] Through closer investigation of those initial alkali phosphorus compounds, a collection of functionalised phosphanes could be isolated to date.[13] The good solubility of phosphanylated aluminates in many commonly used solvents gave great possibilities for many reactions, such as the straightforward phosphanylation of silicon halides.

Major progress for the systematic synthesis and functionalisation of phosphanes was achieved with the isolation of pure, crystalline $LiPEt_2$ by Issleib and Tzschach.[12] This compound, together with other alkali-phosphorus congeners allowed the synthesis of new organophosphorous substances, such as bi- and tri-dentate tertiary phosphanes. Those are of interest because they form very stable complexes with transition metals. The most prominent reported preparations of bidentate tertiary phosphanes are shown in fig.1.5. Metal organophosphides are synthesised *via* metallation of a secondary phosphane, cleavage of triphenylphosphane or reaction of chlorodiphenylphosphane with the metal.[14]

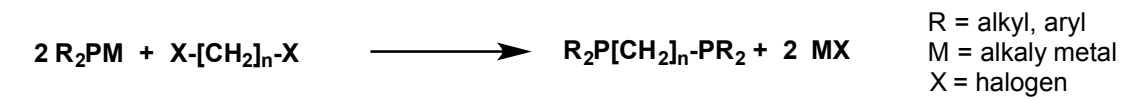


Figure 1.5.: Preparation of bidentate tertiary phosphanes

As mentioned before, synthesis of phosphanes and silylphosphanes through lithium phosphides as phosphide group transfer reagents has proven to be a beneficial method in organometallic chemistry.[15] Therefore, the lithium phosphides have received increasing attention. They often exhibit novel structural features and interesting chemical properties. Since the 1980s, an increasing number of phosphidolithium and bis(phosphido)dilithium compounds have been reported (e.g. **A** in fig.1.6).[15] Just recently ferrocenophan-lithiumphosphanides (see **B** in fig.1.6) were used for embedding heavier tetrylenes into a bridging unit of a [3]ferrocenophane with flanking phosphanyl groups.[16] They were successful in the isolation of a stannylene in the form of a dimeric mutual donor acceptor adduct (see fig. 1.6).

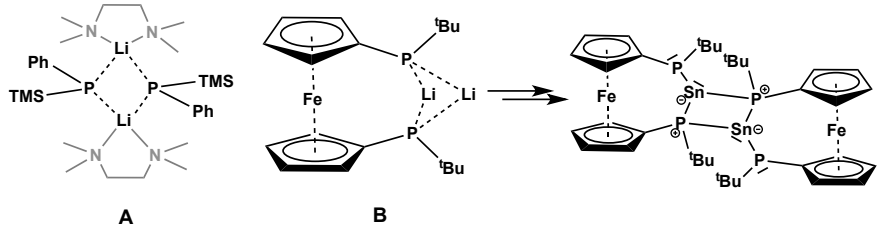


Figure 1.6.: Examples of a tmeda (tetramethylethylenediamine) complexed lithiumphosphanide[15] **A** and a [3]ferrocenophane lithiumphosphanide[16] **B**

Especially the tertiary phosphanes are exceptional ligands towards various metal ions and transition metals.[6] One compound, which has shown tremendous benefits in modern organometallic coordination chemistry, is triphenylphosphane (PPh_3). It is binding well to almost all transition metals and has an average Tolman angle of θ = 145° (PCy_3 = 170° (Cy = C_6H_{11})$_3$) , PMe_3 = 115°).[17] PPh_3 is known for its use in the Wilkinson catalyst, $RhCl(PPh_3)_3$, which has historical significance, since it was used for the hydrogenation of alkenes.[18] This reaction has been widely used in laboratory and industry,[18] making PPh_3 one of the most used compounds for modern

metallorganic chemistry.

Another tertiary phosphane, tris(trimethylsilyl)phosphane, is nowadays highly appreciated in the synthesis of organophosphorus compounds. The chemistry of P-Si molecular compounds has been developed rather late. The first monosilyl phosphanes were isolated in the 1950s by two working groups. Fritz et al.[19] isolated compounds of the type SiH_3PH_2 *via* reaction of SiH_4 with PH_3 while Aylett, Emeleus and Maddock[19] carried out reactions with white phosphorus and SiH_3I to obtain SiH_3PI_2, $(SiH_3)_2PI$ and $(SiH_3)_3P$. After that, reactions of $LiPMe_2$ with chlorosilanes, such as Me_2SiCl_2 or $SiCl_4$ enabled the functionalisation of the first silylphosphanes, $Me_2ClSi\text{-}PMe_2$, $Cl_3Si\text{-}PMe_2$, and $(Me_2P)_2SiCl_2$.

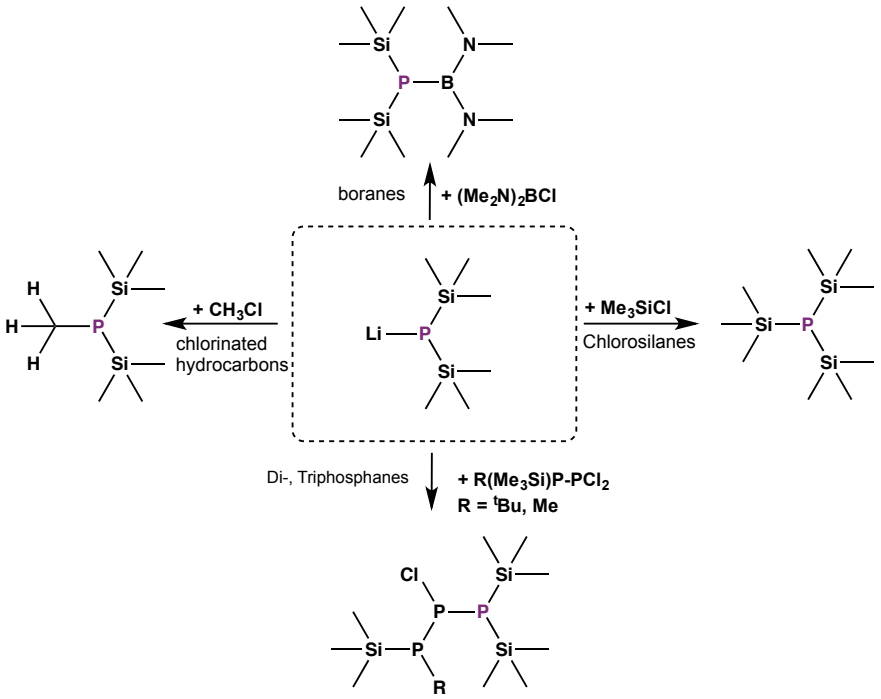


Figure 1.7.: Example reactions of $LiP(SiMe_3)_2$[20] creating numerous organophosphorus compounds

synthesise

Higher substituted silylphosphanes, like the nowadays frequently used $P(SiMe_3)_3$, were used for the synthesis of $LiP(SiMe_3)_2$ *via* the cleavage of Si-P bonds with BuLi. This phosphanide could be reacted with halides and various metals and nonmetals to create numerous organophosphorus compounds

(see fig.1.7).[20] Therefore it is one of todays most used educts in the synthesis of di-, tri-, and tetraphosphanes as well as of cyclic phosphanes with functional groups on the phosphor centres.[20] In 1959 it was possible to synthesise diphenyl(trimethylsilyl)phosphane, the first reported organosilylphosphane, from a reaction of trimethylchlorosilane with sodium-diphenylphosphide.[21] Subsequently, general synthetic pathways for alkylsilylphosphanes, involving the metathesis of alkylchlorosilanes with lithiumphosphides, were investigated by Parshall and Lindsey.[22] Their reactions of trimethylchlorosilane with monolithium phosphide $(LiPH_2)_3$ gave trimethylsilylphosphane $(CH_3)_3SiPH_2$ in about 30% yield. Bubbling the phosphane into a butyllithium solution gave mixtures of di- and trilithium phosphides, again punctuating the difficulties isolating clean silylphosphanes.

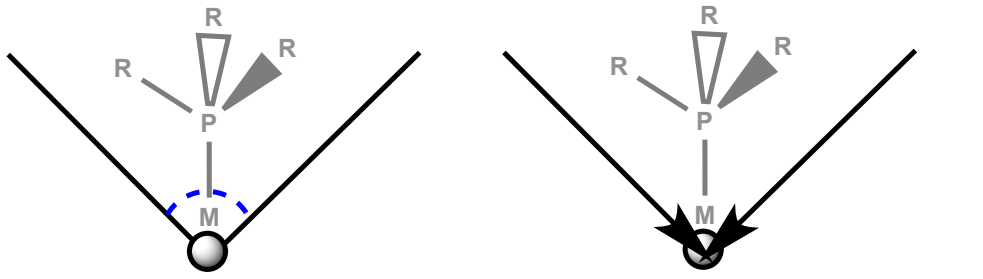
The Si-P bond cleavage is a central topic in the functionalisation of silylphosphanes. As stated in *"The Silicon-Heteroatom Bond"*,[23] silicon-phosphorus compounds are highly reactive. They are readily oxidised, hydrolysed and insert carbon dioxide. Halogens cleave the Si-P bond, with subsequent oxidation to the organophosphorus(V) halide.[23] This can be highly useful in creating novel compounds, e.g. selective ligand systems. The minor stability of the bond however can be problematic for the isolation.

The knowledge about phosphanes and phosphanides has been widely adopted in the functionalisation of silylphosphanes. The 1,2-elimination of Me_3SiCl from silyl-substituted alkylphosphorus chlorides represents a synthetic pathway to compounds containing P=C and P≡C bonds.[24] Since a considerable interest in compounds featuring multiple bonding between heavier main-group elements was developed in the 1980s, the synthesis of silylphosphanes of the type $(Me_3Si)_3SiP(R)Cl$ gained more interest.[25] At this time only one silylhalophosphane, $^tBuP(Cl)SiMe_3$, was reported.[26] This compound however was not stable under ambient conditions. Many attempts to isolate halogenated silylphosphanes have failed due to the facile elimination of silyl halides.[25] Therefore it was necessary to synthesise bulkier silyl systems.

One ligand proved particularly beneficial, the sterically demanding tris(trimethylsilyl)silyl group. The first compounds bearing the $-Si(SiMe_3)_3$ group, hereinafter referred to as hypersilyl or Hyp (a term used by Nils Wiberg[27]) were reported by Gilman et al.[28] Due to its special steric and electronic properties, this ligand can be used to stabilise unusual oxidation states of main group elements and therefore gained more importance in

organometallic chemistry.[27] The hypersilyl moiety provides great steric protection to neighboring groups while generally not being reactive itself, if not specifically targeted.[27] Cowley was able to synthesise the first hypersilyl phosphorus compound, HypP^{t}BuCl.[25]

If talking about ligands in organometallic chemistry, the steric effects around the active metal center, always have to be considered. In the early 1970s, nearly all ligand characteristics were attributed to electronic effects, although steric effects were already contemplated.[29] After that, a number of publications showing the importance of steric effects, it was concluded that they are generally as important as electronic effects.[29] Electronic effects occur if a modification along a chemical bond takes place, in contrast steric effects include forces between molecule parts (usually not bonding) (see fig.**??**ConeAngle2.pdf).[29]



steric = change of bulk of R

R = (**p**-$C_6H_4CH_3$)$_3$ vs R = (**o**-$C_6H_4CH_3$)$_3$

electronic = change of electronic behavior of R

R = (p-C_6H_4**OCH$_3$**)$_3$ vs R = (p-C_6H_4**Cl**)$_3$

Figure 1.8.: Definition of electronic and steric effects[29]

Tolman has quantified the steric bulk of phosphanes with his cone angle method.[10] The cone angle is defined as the apex angle of a cylindrical cone centred 2.28 $\AA$ from the centre of the P atom and just touching the van der Waals radii of the outermost atoms of the molecule (see fig.1.9[29]), providing a picture of the ligand in a frozen state. There are different ways of calculating the cone angle nowadays, which are explained later in the text.

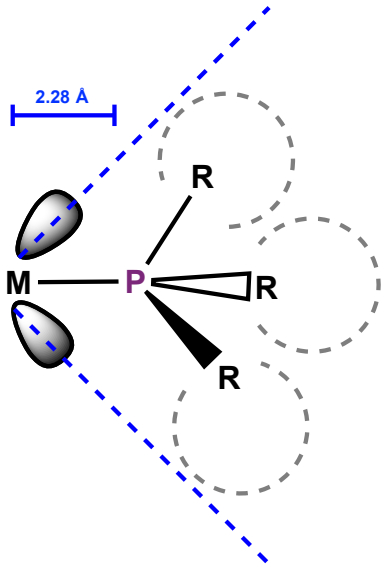


Figure 1.9.: Tolman's cone angle method[10]

1.1.2. Tetrylenes

The steric and electronic effects play a vital role in stabilising carbenes and their heavier analogues. Carbenes are well established compounds in metallorganic catalysis and there is a high number of publications examining the cyclic α,α' - nitrogen stabilised carbenes (*NHC, Arduengo carbene*[30]). Acyclic congeners have, due to their high reactivity, substantial possibilities in transition metal catalysis while still showing enough stability for convenient use. The heavier homologues of carbenes, tetrylenes (M = Ge, Sn, Pb) are able to coordinate to transition metals forming homogeneous catalysts, as is impressively shown in the work of Lappert[31] and Veith.[32] In Lapperts investigations with Pd(II) complexes, Sn[N(SiMe$_3$)$_2$] acts as a two-electron σ-donor, which is a successful alternative to the widely used tertiary phosphanes[33] (see fig. 1.10).

Additionally to their role as ligands, in the last decade investigations have focused on the electronic structure, catalytic ability and reactivity of the heavier carbene homologues. The results have demonstrated that these homologues are monomeric and show no tendency to oligimerise when they have a relatively large S/T separation and bear bulky ligands, which function as intramolecular donor centers.[36] To date, alkyl, aryl, OR, SR, and NR, groups have

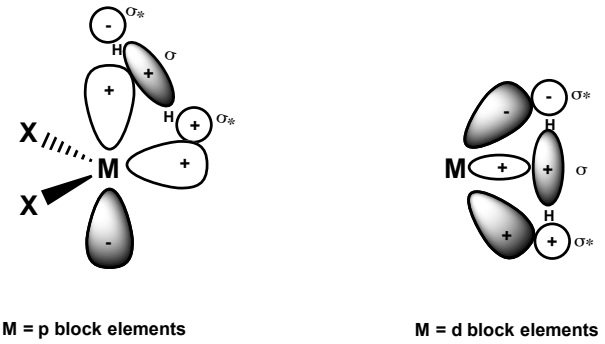


Figure 1.10.: Schematic representations of modes of activation of H_2 at a tetrylene and a transition metal center.[34,35]

been used as the ligand X. The structures of several of these colored, diamagnetic carbene homologues have also been characterised. In order to use the tetrylenes for subsequent chemical reactions, the steric shielding should be small enough to allow access to the reactive tetrel center. At the same time, stability needs to be increased by intramolecular donation of electron density into the empty p-orbital on the tetrel (see fig.1.11).

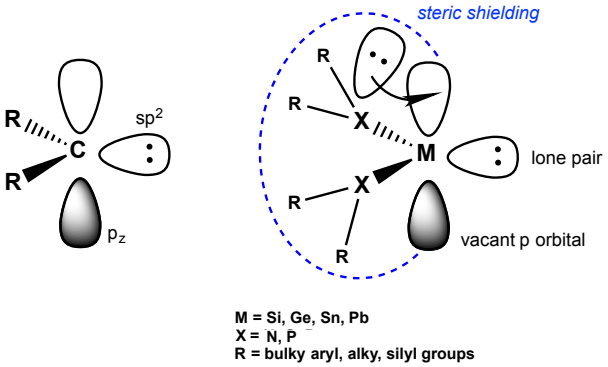


Figure 1.11.: Orbital scheme of singlet carbenes and intramolecular stabilisation of acyclic tetrylenes (left)

Interestingly, compared to the well studied diaminotetrylenes, there is less known about the phosphorus analogues. Despite already in 1996, Schleyer et al.[37] noted that the inherent p-donor capabilities of phosphorus should be as large or even larger than those of nitrogen, still less compounds are known for phosphorus. Thinking of the great variety of phosphane ligands in transition metal complexes, it is curious, that those systems were not used regularly for main group compounds. In diaminotetrylenes, stabilisation is provided *via*

interaction of the group 15 element lone pair with the vacant p-orbital on the group 14 element in oxidation state +II (tetrel atom E = C, Si, Ge, Sn, Pb). Certainly, the difference in the electronegativities (Pauling: N = 3.04, P = 2.19) and the stronger pyramidalisation of the phosphorus might counteract the effective orbital overlap with the empty p-orbital of the tetrel atom. One reason for the small number of diphospha-stabilised tetrylenes was presumed to lie in the large planarisation barrier of the phosphorus atom.[38] Looking at the heavier group 14 analogues, only a few compounds with phosphane ligands on metal centers with M(II) have been reported.[39]

In almost all literature known structures, the P atoms are *de facto* trigonal-pyramidal and no typical planar π -type interactions could be determined. In 1977, the first diphosphatetrylene with the rather small ^{t}Bu substituents, $[(^{t}Bu_2P)]_2Sn_2$, a dimeric compound,[40] was determined *via* NMR spectroscopy. A few years later, the first monomeric structure $(Me_3Si)_2P_2Sn$ was characterised by NMR spectroscopy and cryoscopy,[41] red-orange crystals were isolated, but decomposed while storing at reduced temperature. Since TMS (= $SiMe_3$) and ^{t}Bu are similar in their steric demand, this indicates silyl substituents might be more favourable for the stabilisation of monomeric diphosphatetrylenes compared to alkyl ligands. In 1995 a series of thermally stable, homoleptic tetrylenes of germanium, tin, and lead was isolated by Driess.[36] All compounds bear rather bulky, sterically demanding silyl substituents, -Si(2,4,6-$^{i}Pr_3C_6H_2)_2F$ and Si(^{t}Bu)(2,4,6-$^{i}Pr_3C_6H_2)F$, on the pyramidal phosphorus atom (fig.1.12).

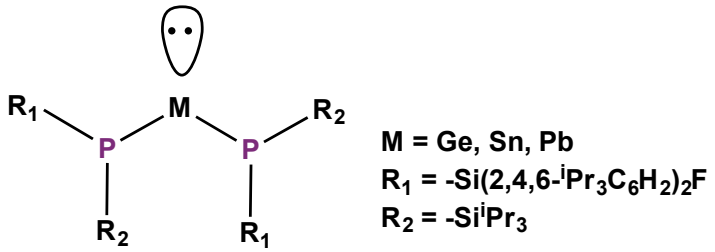


Figure 1.12.: Isolated diphosphatetrylenes[36] with bulky silyl ligands

Also bulky phospholide substituents and aromatic systems, $[Ar^{Mes_2}P(Ph)]_2Sn$ (Ar^{Mes_2} = C_6H_3-2,6(C_6H_2-2,4,6-Me_3)), were used in the stabilisation of diphosphastannylenes, shown by Westerhausen in 1998 and Rivard[42] in 2007. Stabilisation *via* formation of phosphastannenocenes was also mentioned

by Brym and Jones.[43] In 2005 and 2012, comparatively small, diphosphatetrylenes, $[(Me_3Si)_2\text{-}CH]P(C_6H_4\text{-}2\text{-}SMe)_2E$ (E = Ge, Sn) and $[(Ph)(C_6H_3\text{-}2,6\text{-}CH_2NMe_2)_2P]_2Sn$ were isolated by Izod[44] and Řezníček.[45] In both cases, additional stabilisation of discrete monomers was reached by intramolecular base stabilisation *via* a sulphur or a nitrogen lone pair.

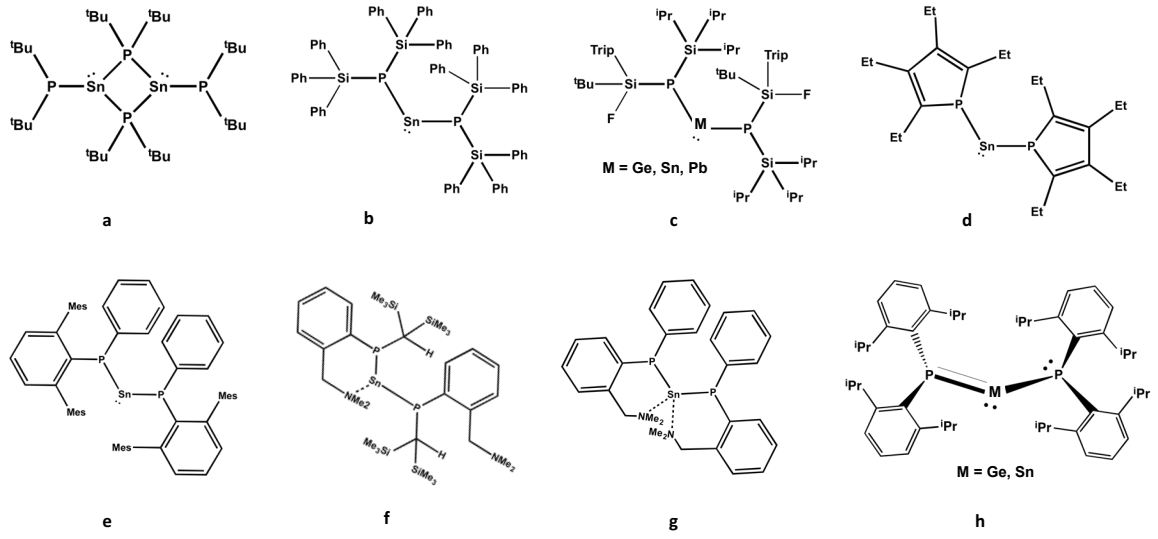


Figure 1.13.: A selective overview of acyclic diphosphatetrylenes to date **(a,[40] b,[46] c,[36] d,[47] e,[42] f,[48] g,[45] h[49])**

All of the above mentioned and literature known monomeric diphosphatetrylenes feature rather bulky and sterically demanding alkyl, aryl, or silyl substituents[47] on the pyramidal phosphorus atoms. Until now there is only one ”free” diphosphagermylene fully characterised. The compound, $(Dipp_2P)Ge$ (Dipp = $(2,6\text{-}^iPr_3C_6H_2)$), is the first diphosphatetrylene stabilised *via* $p\pi$ - $p\pi$ interactions with a trigonal-planar phosphorus center (fig.1.13).[38]

As suggested by Izod, stabilisation in diphosphatetrylenes could be fortified by a strong P=E multiple bond character.[49] Such a strong intramolecular stabilisation could allow the use of smaller substituents for stable tetrylenes. However, what is missing is an understanding in what factors of the ligand including substituent size, steric demand and kind of substituent (aryl, alkyl, silyl), affect isolation and stabilisation of novel compounds.

The key to success for the stability of diphosphatetrylenes, should be the determination of substituents that provide sufficient steric protection, together with decreasing the pyramidalisation of the P-atom to obtain optimal orbital overlap. Therefore a closer examination of various phosphanes and phosphanides and their possible use in main group chemistry is necessary.

1.1.3. Silylboranes

Silylboranes have gained increasing importance in recent years, mainly as substrates for transition metal catalysed silylation reactions.[50] Just recently, contemporary calculations showed that stabilisation in H_2/BR_2 (R = silyl ligands) complexes can be provided in a similar way as in transition metal complexes,[51,52] enabling various catalytic possibilities in metalorganic chemistry.[53]

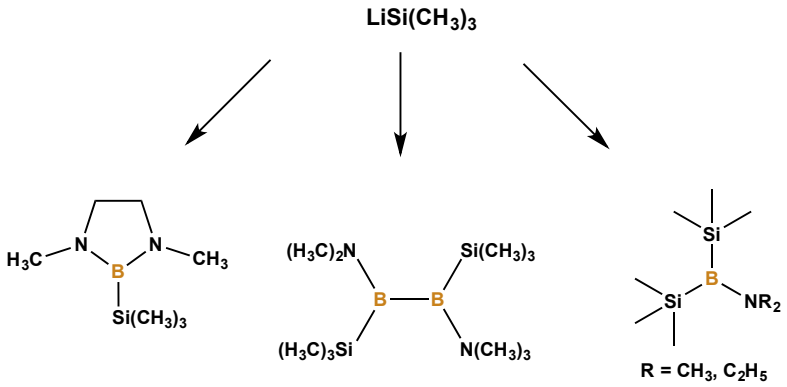


Figure 1.14.: Silylborane studies performed by Nöth[50]

The first silylboranes were synthesised in 1960s, despite this long history of silylboranes, few systematic studies of their reactivity are available.[50] The most extensive studies were performed by Nöth, who prepared B-Si compounds which contain an (electronically shielding) B-N bond. Similar to stabilisation of tetrylenes, where electron density is donated into the free orbital of the tetrel atom, donating electron lone pairs of N, P, or O are used in the stabilisation of silylboranes. The reaction of $(CH_3)_3SiLi$ with various boron compounds led to their functionalisation. For example the reaction to 1,2-dimethyl-2-trimethylsilyl-1,3,2-diazaborolin, or the reaction to diboranes and the reaction of dichloro(dimethylamine)borane with $(CH_3)_3SiLi$ to the double silylated dimethylaminobis(trimethylsilyl)borane.[50] (see fig.1.14).

Conversely to silylphosphanes, silylboranes are most commonly prepared by reaction of silyl anions with boron halides. The reaction is limited, because the resultant silylboranes easily add an equivalent of the silicon nucleophile to form the corresponding anionic tetracoodinated borate. This can be hindered by steric or electronic shielding of the boron.
In 2004, a reaction pathway for the reaction of tris(trimethylsilyl)silyl potassium with piperidinodichloroboranes and dichlorophosphanes was successful in the formation of phospha- and boracyclopentasilanes (see fig.1.15).[52]

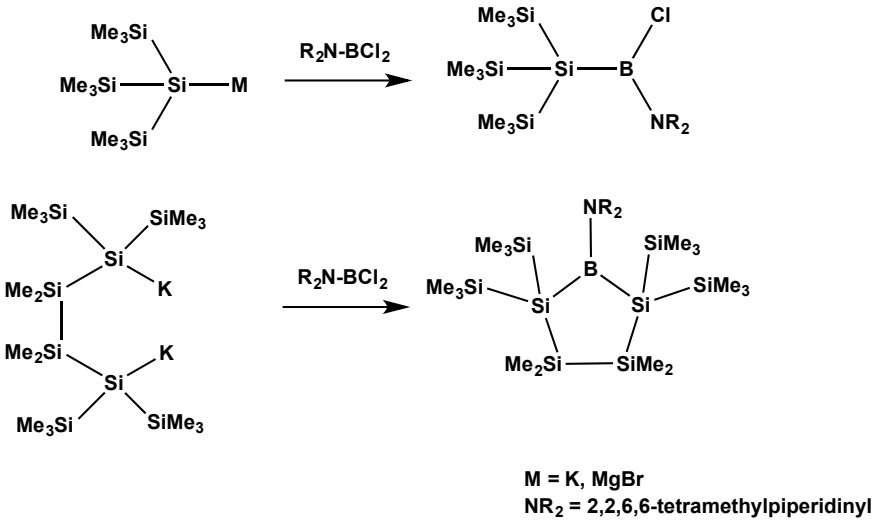


Figure 1.15.: Reaction pathways for acyclic and cyclic silylboranes form silyl anions[52]

However, since the amount of publications containing silylboranes is quite small, a more precise synthetic investigation is necessary. Double silylated boron compounds might be promising intermediates in the synthesis of trisilylated boron compounds, which are still quite unexplored in organosilicon chemistry. Therefore during this work various alternative reaction pathways for the isolation of stable silylated boranes were explored.

1.2. Theoretical methods

Molecular modelling is a powerful tool to estimate how various substituents influence the geometric structure and stabilisation of compounds. This makes it possible to estimate what compounds are suitable for synthesis. During this

thesis various phosphanes, boranes and low valent group 14 compounds were investigated *via* DFT.

1.2.1. Basics of DFT

This introduction is based on Peter W. Atkins' "Physikalische Chemie",[54] "Essentials of Computational Chemistry-theories and models" by Christopher J. Cramer,[55] Neil S. Ostlund's "Modern Quantum Chemistry",[56] "Quantum Chemistry" by Ira N. Levine[57] and parts of prior summarised work.[58]

Density functional theory (DFT) provides a powerful tool for computation of the quantum state of atoms, molecules and solids, and of ab-initio molecular dynamics. The foundation stone of todays DFT was the approximate version of Thomas and Fermi after the foundation of quantum mechanics in 1927. After that, Hohenberg, Kohn and Sham established the new DFT in the 1960s with their work "Inhomogeneous Electron Gas".[59] Today, the DFT is the most commonly used method for the calculation of molecular structures.[59]
The central parameter of the DFT is the electron density ρ instead of the wave function Ψ. The term "'functional"' in Density Functional Theory comes from the fact that the energy of the molecule is a function of the electron density $E_{[\rho]}$.[54] The electron density is a function of location, $\rho=\rho(r)$ and a function of a function is called functional. The energy of the ground state is described as follows.[54]

$$E_{[\rho]}=(E_{kin}+E_{p,EK}+E_{p,EE}+E_{p,Aus})[\rho] \tag{1.1}$$

E_{kin} is the kinetic energy of the electrons, $E_{p,EK}$ the potential energy of the electron-nuclear attraction, $E_{p,EE}$ the potential energy of the electron-electron repulsion and the exchange-correlation energy $E_{p,Aus}$, which takes all effects due to the spin in account.[54] The orbitals can be calculated from the Kohn-Sham equations. The electron density can be determined by applying equation (1.2). To determine the electron density, the Kohn-Sham functions Ψ_i, which are *n* solutions of the Schrödinger-equation in an effective potential function

v_{eff} were set off. The density is obtained from the sum of the electron densities of the Kohn-Sham equations:

$$\rho = \sum_{i=1}^{n} |\Psi_{\text{i}}(\vec{r})|^2 \tag{1.2}$$

The effective potential is dependent on the density:

$$v_{\text{eff}} = v(\vec{r}) + \int \frac{n(\vec{r})}{|\vec{r} - \vec{r}|} d^3r' + v_{\text{xc}}(\vec{r}) \tag{1.3}$$

Here the first term, $v(\vec{r})$, is the external potential which substantially describes the attraction of the electrons by the atomic nuclei, and the second term describes the electrostatic interaction of the electrons with each other (Hartree-term). The solutions of the equations must be found iteratively, since the effective potential $v_{\text{eff}}(\vec{r})$ is dependent on the density $\rho(\vec{r})$ which itself is dependent on the solutions of these equations.[54] The third term $v_{\text{xc}}(\vec{r})$ is the so-called exchange correlation potential ("x", "exchange", "c" for "correlation") which ensures the correct treatment of multielectron systems.
A start-electron density is assumed, usually a simple superposition of the atomic electron densities. Then, the exchange-correlation potential is calculated. With this potential the Kohn-Sham equations can be solved to obtain a new potential. With this information it is possible to obtain a better approximation for the electron density. This process is repeated until a stable (self-consistent) solution is found.
The Kohn-Sham functions are pure calculation values and have no physical meaning by itself. Strictly speaking $v_{\text{eff}}(\vec{r})$ is dependent on the electron density at all sites and not just at the point $\vec{r}$, and can be calculated accurately for very few trivial cases. However, in practice this approach can often be used as an approximation of actual electron states. With DFT calculations, it is possible to determine the total energy of the atomic configuration. This, for example, can be helpful to find the most energetically favorable of several possible arrangements of a compound.

For the calculation, the choice of the right functional turns out to be of great importance, there is a multitude of different kinds of functionals with specific characteristics for each type of calculation. It has become evident, that for most calculations a hybrid functional, which includes a proportion of classical

Hartree-Fock calculation, produces better results than those based only on the electron density. Hybrid DFT is mixing various amounts of Hartree-Fock (HF) nonlocal exchange operator with DFT exchange correlation functionals.[60] Among these mPW1PW91 has proven to accurately reproduce molecular structures, vibrational frequencies, and bond energies.
The fraction of HF exchange is set to 25% in mPW1PW91.[60] Recently, double hybrid functionals have emerged that are most reliable for thermochemistry and non-covalent interactions.[61,62] Calculations, both for covalent and non-covalent interactions, are possible in a satisfactory theoretical framework encompassing the free electron gas limit and most of the known scaling conditions.[63]

The choice of the compatible basis set is even more convoluted. A basis set is a set of functions, which is used to represent the electronic wave function in the HF method or DFT. Orbitals are wave functions, one-electron functions, eigenfunctions of an eigenvalue problem, the Schrödinger-equation for example, that describes the behaviour of an electron in three-dimensional space. These orbitals have no physical meaning, can have positive and negative values in different spatial areas and can, in principle, also be complex. By the linear combination of functions, which should represent the orbital as well as possible, orbitals in atoms and molecules can be described mathematically.

$$\Psi_{\mathrm{i}} = \sum_{r} c_{\mathrm{ir}} \phi_{\mathrm{r}} \quad (LCAO - method) \tag{1.4}$$

Originally the molecular orbitals were, according to the LCAO-method (LCAO = Linear Combination of Atomic Orbitals), approached by an actual linear combination of atomic orbitals.
It is common to represent valence orbitals by more than one basis function, where each of which can be composed of a fixed linear combination of primitive Gaussian functions. Split valence basis sets, such as 3-21G and 6-31G basis sets, have two (or more) sets of basis functions for each valence orbital. Since the different orbitals of the split have different spatial extents, the combination allows the electron density to adjust its spatial extent appropriate to the particular molecular environment.

For a description of weakly bound electrons, such as anions, diffuse basis functions are required. An example of a basis set with diffuse basis functions is the 6-31+G.[64] Polarization functions, are functions with an additional node and allow a better description of charge polarization. They are denoted by a * or a *d* (d-type functions added to atoms; f-type functions added to transition metals). Relativistic effects increase with heavier elements. Calculations become more complicated and demanding in larger systems. This results in a natural enlargement of the required basic set. For example, 35 electrons and their orbitals must be described for a bromine atom. In order to reduce the computational effort, without great loss in the quality of the results, a method introduced by Hellmann in the 1930s can be used.[65]This is based on treating the near-nuclear, full-orbital electrons separated from the valence electrons. These electrons of the inner shells change only minimally with the chemical environment, and can therefore be described by an effective potential. From a certain distance to the core, the potential corresponds to the ”cut-off radius”, the actual course of the potential curve. Effective core potentials (ECPs) are used to replace the inner (core) electrons of atomic and molecular systems by an effective potential and treat only the valence electrons explicitly in quantum mechanical calculations. This leads to substantial reductions in computational effort and also allows for an efficient treatment of relativistic effects.[66] Correspondingly ”small-core” and ”large-core” ECPs are available for a variety of elements.[66] Most frequently used examples of ECPs in computational chemistry are LANL2DZ[67] and Stuttgart-Dresden (SDD),[67] which was used during this work.

1.2.2. Applications of DFT calculations

Apart from the prediction of structures, stabilities and reactivities, DFT calculations can be used to predict spectra and help the peak assignment. Today the most widely used method to calculate excitation energies and electronic spectra is time-dependent DFT (TDDFT).[68] With time-dependant DFT the singlet electron excitations can be obtained. This information makes it possible to predict the colour of the calculated molecule, which has been proven to be accurate for a wide range of compounds.[68] The interpretation of the calculated excitation energies is an important point for the connection of synthesis

and calculation of molecules. Knowledge of the estimated color of the desired product can be a big advantage in the synthesis.

To analyse geometries and electronic structures of molecules, NMR calculations can be a helpful tool.[69] The information obtained by an NMR calculation is the magnetic shielding of the nuclei. To compare the calculated shifts with the measured NMR data, one must calculate the magnetic shielding of the reference molecule (TMS for ^{1}H, ^{13}C, and ^{29}Si and PH_3 for ^{31}P).
This magnetic shielding is mathematically proportional to the second derivation of the energy change between the states with existing or absent external magnetic field. A magnetic field does influence the kinetic energy operator.
However, the grade of influence depends on the coordinates, so it is necessary to determine the origin of the coordinate system somewhere in the molecules. A magnetic field that acts from outside during an NMR experiment on a molecule is in this respect location-independent.
The dependence of the calculated shifts of location brings, except under very special conditions, incorrect results. These conditions include either the calculation of the exact wave function or the use of an infinitely large basis set, which is not possible in practical computational chemistry.
It is common to use the GIAO (”gauge invariant / independent atomic orbitals”)[70] approach. It is based on compensating the spatial dependence of the kinetic energy with the basic functions, which makes every calculated core to an origin and therefore location-independent. This approach is generally used and was also resorted to in this work it.
For our calculations, the M06-L meta-GGA (generalized-gradient-approximation) has proven to be a helpful tool in predicting NMR shifts for the synthetic approach. It was designed for main group thermochemistry, transition-metal bonding, thermochemical kinetics and noncovalent interactions.[71] It has shown to give good performance calculating magnetic shifts and coupling in organic and inorganic molecules.[71]
The calculated NMR shifts deviate in average 15 % from the experimental data. The correct calculation of nuclear magnetic shielding constants is an active research area in computational chemistry.[71]

1.2.3. Calculation of cone angles

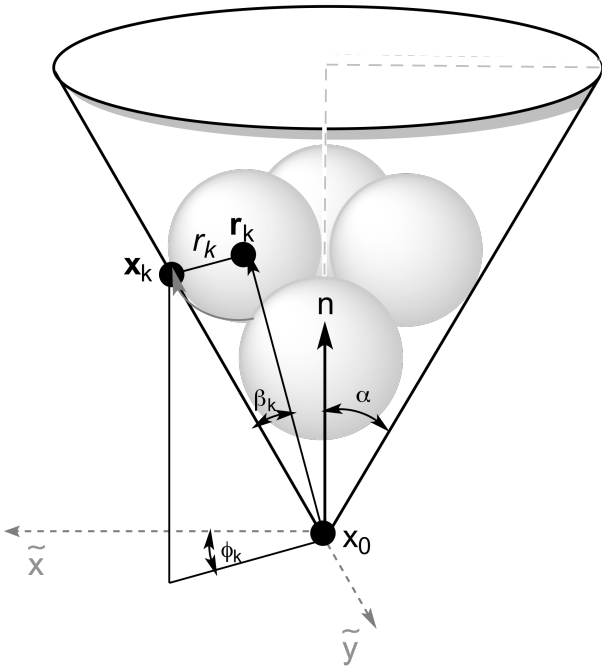


Figure 1.16.: Parameters for determining the exact cone angle[1]

Steric bulk of ligands is usually determined by Tolman θ or solid cone angles Θ,[1] which both suffer from some disadvantages such as the imprecision with asymmetric and polydentate ligands or for the solid angles, only providing a picture of the ligand in a frozen state.[1] In contrast the ”exact cone angle method”[1] is a more convenient technique for determining exact cone angles θ° *via* finding the most acute circular cone, containing all ligand atoms over a quadratic equation for the cosine of the cone angle. The size of the cone angle describes the ability of shielding an active metal centre. Commonly used phosphane ligands show values around 200°[72] . The only necessary information, are the Cartesian coordinates of the metal centre and the ligand atoms, which should be provided by crystallographic structures or quantum chemical geometry opitimisation.[1]

In the first description of the method, the exact cone angle is defined as the apex angle (2α) of the most acute right circular cone that originates at the metal centre and contains all ligand atoms. Each atom of the ligand is described by

a sphere centred at $\mathbf{r}_k$ (fig.1.16) with the van der Waals radius r_k. The location x forming the surface of a right circular double-cone with apex at x_0 and axis along unit vector **n** is given by:

$$\frac{(x - x_0) \cdot n}{|x - x_0|} = \pm cos\alpha \tag{1.5}$$

The cone contains all atoms in the ligand and is tangent to one, two or three of the ligand atoms, dependent on the spatial arrangement of those. Each atom correnspponds to a tangent point (x_k), which is coplanar with the atom centre ($\mathbf{r_k}$), metal centre(x_0) and the cone axis y(t). To ease calculations, body fixed coordinate-systems are used, expressed with tildes (fig.1.16), with the origin at the apex and the cone axis n directed along the z axis.[1]

If the cone is located only by a single atom k, then θ° = 2 α_k = 2 β_k, and the cone axis **n** is directed along m_k. If the cone is determined by two atoms *a* und *b*, the cone angle is simplified expressed by:

$$\theta^\circ = 2\alpha_{ab} = \beta_{ab} + \beta_a + \beta_b \tag{1.6}$$

The exact cone angle method gives cone angles approximately 25° larger than reported Tolman cone angles, however the method used by Tolman underestimates steric demand for phosphine ligands.[1] Calculated cone angles with the exact cone angle method rather resemble values calculated from crystallographic data.[1]

1.3. Scope of the work

The aim of this work is to design, synthesise and characterise silylphosphanes as possible ligands for the formation of P, P' stabilised germylenes and stannylenes. Phosphanes with aryl, alkyl and silyl substituents on the phosphorus atoms were investigated in a DFT study, to identify ideal phosphane ligands for the preparation of stable tetrylenes. Calculation of spectral properties will help in the assignment. These molecules are of interest due to their ability to activate small molecules, such as as H_2, NH_3 or CO_2.

In line with tetrylenes, silylboranes could feature similar characteristics. Di- and trisilylboranes with bulky silyl groups, such as the Hyp, are still rare. Therefore novel methods should be developed to synthesise and isolate these scarce, but highly interesting compounds.

Chapter 2

Results and Discussion

To better understand the stabilisation of low valent compounds, DFT calculations and experimental investigations on various phosphanes and phosphanides were explored. Through these considerations, ligand systems capable of isolating stable low valent main group 14 species, were determined.

2.1. Theoretical investigation of phosphane ligands

As stated before, the design of ligands is an important tool in organometallic chemistry, because ligands can be fitted to specific requirements in synthesis. Phosphane ligands have already proven their versatile applicability. However there is still just a small number of diphospha stabilised compounds known. This is attributed to the pyramidalisation of the P atoms, which is assumed to cause smaller orbital overlap and therefore less stable compounds as comparable nitrogen compounds. In those the characteristics of binding are different, because nitrogen compounds can be planar, also the nitrogen atom is smaller (N $r_{atom(kov)}$ = 0.70$\mathring{A}$, P $r_{atom(kov)}$ = 1.10 $\mathring{A}$) and has a higher electronegativity (N = 3.04, P = 2.19 (Pauling)). Within a DFT study, it was confirmed that the inherent p-donor capabilities of phosphorus should be as large than those of nitrogen.[37]

Phosphanes with aryl, alkyl and silyl substituents on the phosphorus atoms were investigated in a DFT study. Greater focus was placed on $PhPR_2$,

Table 2.1.: mPW1PW91/SDD DFT calculated geometry data and ^{31}P NMR shifts for different phosphanes

Compound	$\sum$ P(P') [°]	P-C [$\AA$]	P-R [$\AA$]	^{31}P NMR$_{calc.}$ [ppm]	^{31}P NMR$_{exp.}$ [ppm]
PhPR$_2$					
Substituent R					
H	289.4	1.88	1.44	-122.8	-124.7[73]
Me	299.9	1.88	1.89	-34.2	-46.5[74]
^{t}Bu	318.0	1.88	1.95	-45.6	-40.2[75]
TMS	313.4	1.88	2.34	-113.7	-133.5[76]
Hyp	324.7	1.89	2.39	-80.6	-132.9[i]
Ph	305.1	1.87	1.87	-3.2	-4.7[75]
Mes*PR$_2$					
H	293.4	1.90	1.44	-124.1	-132.4[77]
Me	319.9	1.89	1.89	-24.5	
^{t}Bu	341.8	1.90	1.96	-55.9	
TMS	351.9	1.89	2.34	-113.1	-146.0[i]
Hyp	359.9	1.90	2.48	-109.4	
Ph	326.3	1.86	1.87	-3.1	
HypPR$_2$		**P-Si [$\AA$]**			
H	287.0	2.36	1.44	-235.8	-265.4[27]
Me	303.1	2.36	1.90	-76.8	
^{t}Bu	321.5	2.41	1.95	-57.1	
TMS	333.1	2.36	2.35	-221.2	-268.8[27]
Hyp	341.7	2.43	2.49	-	
Ph	312.1	2.38	1.88	-26.6	

[i]see experimental part

Mes*PR$_2$ and HypPR$_2$ with R = H, Me, ^{t}Bu, TMS, Hyp and Ph, as ligand systems for the isolation of novel compounds. Those are comparable to substituents used in literature known compounds and will therefore give a great outline of the ligand features.

Looking at the calculated data for the phosphanes, we can detect a trend in the pyramidalisation of the phosphorus atom. A substitution with ^{t}Bu, TMS and Hyp has a greater influence on the pyramidalisation of the phosphorus atom than substitution with the comparatively small H or methyl group. Mes* substituted phosphanes, seen in Table 2.1, appear particularly suitable for lowering the pyramidalisation of the P atom. This effect is stronger if together with Mes* there is a silyl group attached to the P atom. Although the TMS group is isomorphic[78] and similar in size to the ^{t}Bu ligand, the bond angle sum (ΣP) increases

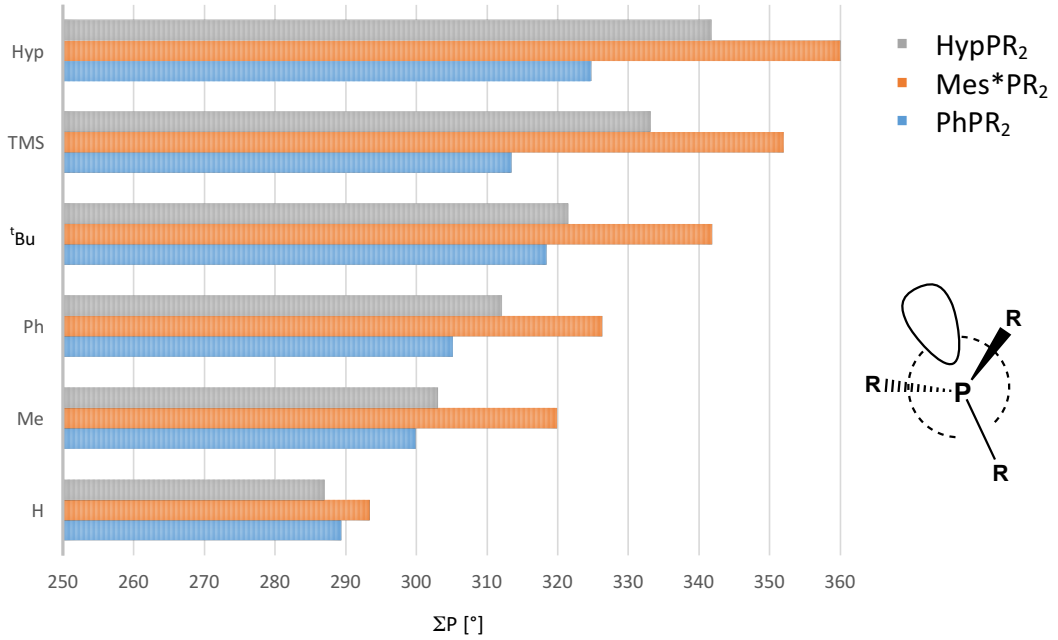


Figure 2.1.: Planarity Σ P [°] of the P atom with various substituents

by 10 degrees going from ^{t}Bu (ΣP = 341.8°) to TMS (ΣP = 351.9°). The combination Mes*PHyp$_2$ provides an angle sum of 359.9°, understood as planar conformation (fig.2.1). A threefold substitution with Hyp also gives an almost planar P, however experimental accessibility of this compound is hardly possible, due to the high steric bulk.
But for stabilisation of tetrylenes not only the effective orbital overlap has to be considered in terms of stabilising effects, but the steric demand of ligands has to be examined as well. The bulk of ligands is usually quantified with calculating the cone angle. Commonly used phosphane ligands show values around 200°.[72] Using the exact cone angle method,[1] we calculated values for the Dipp and Tripp substituents, which were recently used by Izod[38,49] for the synthesis of stable diphosphatetrylenes. Those have cone angles of 204° to 205°. In Table 2.2 the DFT calculated data of the P atoms, attached to heavy atoms and with ligands from small, H, to bulky, Hyp, are summarised together with their exact cone angles.

The shielding of the active centre E (E = Ge, Sn), seems especially good for silyl substituted phosphane ligands in low valent compounds. Values in between 180° and 200° could be obtained. H, Me and Ph substituted

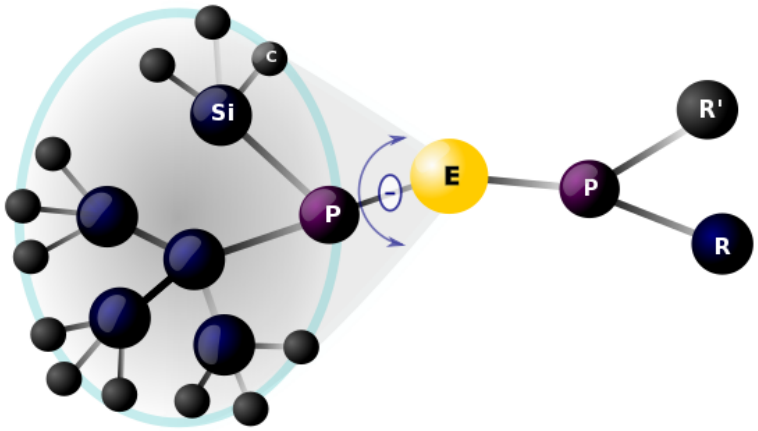


Figure 2.2.: Schematic diagram of diphosphatetrylene cone angles

Table 2.2.: mPW1PW91/SDD DFT calculated geometry data and exact cone angles for homoleptically tetrylenes (E = Ge, Sn)

Compound	$\sum$ P(P') [°]	P-R/P'-R [$\AA$]	P-E/P'-E [$\AA$]	P-E-P [°]	**Cone Angle** θ°
$(PR_2)_2Ge$					
Substituent R					
H	307.3(307.5)	1.43/1.43	2.43/2.42	94.5	89
Me	317.2(317.1)	1.89/1.89	2.41/2.40	91.6	120
^{t}Bu	306.3(355.0)	1.94/1.96	2.52/2.32	100.5	180
TMS	304.7(360.0)	2.34/2.35	2.49/2.31	96.0	175
Hyp	314.1(357.2)	2.52/2.69	2.69/2.52	117.1	201
Ph	294.8(360.0)	1.88/1.88	2.52/2.31	95.9	138
$(PR_2)_2Sn$					
H	302.8(302.8)	1.44/1.44	2.61/2.61	91.3	99
Me	316.3(316.3)	1.90/1.90	2.60/2.60	92.1	114
^{t}Bu	308.5(351.1)	1.94/1.95	2.69/2.52	98.9	153
TMS	312.3(348.0)	2.34/2.32	2.64/2.51	93.8	177
Hyp	317.3(358.9)	2.57/2.71	2.71/2.57	118.0	202
Ph	284.2(321.1)	1.87/1.87	1.87/1.87	97.0	121

phosphanes are, with values from 89° to 120°, less suitable. Interestingly, comparing (^{t}Bu)$_2$P$_2$Ge and (^{t}Bu)$_2$P$_2$Sn, a quite remarkable difference in the cone angles (180° and 153°) can be determined. In both, germylenes and stannylenes the highest values for the cone angle were determined for the Hyp substituted compounds, which therefore might be an effective ligand for isolating stable compounds. For all other investigated systems, the steric bulk is too small to prevent further reactions, such as dimerisation.

Planarity is discussed to play a key role in the achieving the affective orbital overlap, an ideal donation of electron density of the P atoms into the empty p orbital of the tetrel atom, seen at planar nitrogen conogeners (diaminotetrylenes). Therefore planar P centres should be more favourable. Our DFT calculations revealed, that especially systems bearing ^{t}Bu, TMS or Hyp groups on the P atoms have conformers with one planar and one pyramidal P centre. The calculations further have demonstrated, that ligands substituted with the comparatively small H, Me and the rigid Ph group, seem less suitable for lowering the pyramidalisation.
NBO analysis showed that in conformers with one planar P centre strong π -type interactions occur. At the same time, the second P centre is considerably weakened expressed by an elongation of the P-Sn bond. As seen in (^{t}Bu)$_2$PSn, with one planar and one pyramidal P centre, with an elongated P-Sn bond of 2.69 $\mathring{A}$.
Consequently steric shielding needs to be increased to ensure stabilisation. In case of two pyramidal P centres, simultaneous interaction between the lone pair of both P centres with the empty p orbital of the Sn is found, but yields comparably low delocalisation energies. A restricted scan for the planarisation of one P centre of the stannylene of type (Ph)$_2$PSn shows a very small barrier of approximately 5 kJ/mol.

Since literature known compounds are either substituted with bulky aromatic, alkyl and silyl substituents, we wanted to explore a combination of those substituents, leading to heteroleptically substituted compounds. These give the possibility of more variable ligand combinations and therefore increasing utilisation. Since calculations for homoleptic substitution showed benefits for R =

Table 2.3.: mPW1PW91/SDD DFT calculated data for heteroleptic substituted tetrylenes (E = Ge, Sn

Compound	$\sum$ P(P') [°]	P-R/P'-R [$\AA$]	P-E/P'-E [$\AA$]	P-E-P [°]	**Cone Angle** θ°	$\Delta_{\text{H-L}}$ [eV]
$(PhPR)_2Ge$						
Substituent R						
^{t}Bu	326.4(321.9)	1.95/1.95	2.39/2.40	103.0	149	3.40
TMS	313.4(313.6)	2.36/2.36	2.41/2.41	94.4	142	3.45
Hyp	340.9(302.4)	2.34/2.37	2.36/2.48	102.7	180	2.85
$(PhPR)_2Sn$						
^{t}Bu	306.7(347.8)	1.95/1.93	2.66/2.51	90.76	153	2.94
TMS	314.3(314.1)	2.35/2.36	2.60/2.60	91.20	143	3.45
Hyp	328.5(328.6)	2.36/2.36	2.58/2.58	99.74	178	2.96
$(Mes^*PR)_2Ge$						
Substituent R						
^{t}Bu	322.2(359.9)	1.99/1.98	2.52/2.32	104.2	175	3.03
TMS	346.5(359.9)	2.35/2.35	2.40/2.33	113.3	173	2.98
Hyp	331.5(359.9)	2.40/2.38	2.67/2.53	112.1	202	2.89
$(Mes^*PR)_2Sn$						
^{t}Bu	325.4 (360.0)	2.00/1.98	2.70/2.52	104.2	178	3.05
TMS	347.0 (360.0)	2.34/2.35	2.35/2.36	110.3	176	3.25
Hyp	331.5 (359.9)	2.38/2.40	2.61/2.56	112.1	201	3.03
$(HypPR)_2Ge$						
Substituent R						
^{t}Bu	307.9(359.8)	1.96/1.94	2.51/2.32	103.0	199	4.47
TMS	328.5(328.5)	2.35/2.35	2.41/2.41	102.2	198	2.70
$(HypPR)_2Sn$						
^{t}Bu	309.7 (360.0)	1.96/1.94	2.68/2.51	102.0	198	3.16
TMS	328.0 (328.0)	2.35/2.36	2.58/2.61	98.82	197	3.11

^{t}Bu, TMS and Hyp, heteroleptic systems with the base structures phenylphosphane ($PhPR_2$), supermesitylphosphane (Mes^*PR_2) and hypersilylphosphane ($HypPR_2$) (see Table 2.3).

Starting with the smallest base **$PhPR_2$**, more than one stable conformation of every ligand combination $(PhPR)_2E$ (R = ^{t}Bu, TMS, Hyp; E = Ge, Sn) could be calculated. In case of the **^{t}Bu** substituted germylene the global minimum structure has two pyramidal P centres. The P-Ge-P angle is 103.0° and the P-Ge bonds are the same length (1.95 $\AA$). There is also a minimal structure with a planar P centre, which is 5.5 kJ/mol less stable. In the stannylene, the global minimum structure has one almost planar and one pyramidal centre (see fig.2.3). In this case there is another minimum similar in energy, $\Delta H_{rel} < 1$

kJ/mol difference (0.96 kJ/mol), which is quite symmetric and has 2 pyramidal centres. The global minimum shows a rather small P-Sn-P' angle of 90.76°. Such small bond angles were also detected in literature known compounds with aromatic substituents. Izod[49] isolated [(2,4,6- $^{i}Pr_3C_6H_2)_2P]_2Sn$ with an P-Sn-P' angle of 89.62°. In those compounds structures with planar P centres were isolated, however a rather small energy barrier between the conformations was detected. In solution both conformers are in a dynamic equilibria. The global minimum of $(PhP^{t}Bu)_2Sn$ has P-Sn bond lenghts of 2.66 $\AA$ and 2.51 $\AA$ long, the shorter bond at the planar centre.

For the **TMS** substituted compounds, we can find four minimum structures. For $(PhPTMS)_2Ge$, three of those are quite similar in energy ($\Delta H_{rel} < 3$ kJ/mol), and have two pyramidal P centres, only one does have one almost planar centre. This conformer however is 15 kJ/mol less stable than the global minumum. The minimum structures of the TMS substituted stannylene $(PhPTMS)_2Sn$, are as well rather similar in energy. Three have two pyramidal P centres, only one compound, which is also the least stable conformation, has a planar P centre. The P-Sn-P' angle of the global minimum is with an value of 91.20° comparatively narrow.

For the **Hyp** substituted compounds, presently only one stable conformation of $(PhHypP)_2Ge$ could be calculated, this compound has two pyramidal centres, one is slightly flatter ($\sum$ P(P)' = 340°), reflected in the bond lengths of 2.48 (pyramidal centre) and 2.36 (more planar centre). The P-Ge-P is with 102.7° slightly wider than in the corresponding tin compound. For $(PhHypP)_2Sn$ four stable structures could be determined, all of them are similar in energy. Three conformations have two pyramidal centres only one has a planar P centre, this conformer is 0.06 kJ/mol less stable than the global minimum. It has a P-Sn-P' angle of 102.9°, again with a shorter bond (2.51 $\AA$) at the planar centre.

Starting from the slightly bulkier aromatic base structure **Mes*PR$_2$**, four stable minimum structures are found for the **^{t}Bu** substituted compounds. $(Mes^*P^{t}Bu)_2Ge$ has three conformers with one pyramidal and one planar phosphorus centre. For this molecule one miniumum structure is found with two almost planar P centres (352.1/352.2), this conformer however is 37 kJ/mol less stable (see fig.2.4). Obviously, planarisation of both P centres is energetically rather unfavourable.

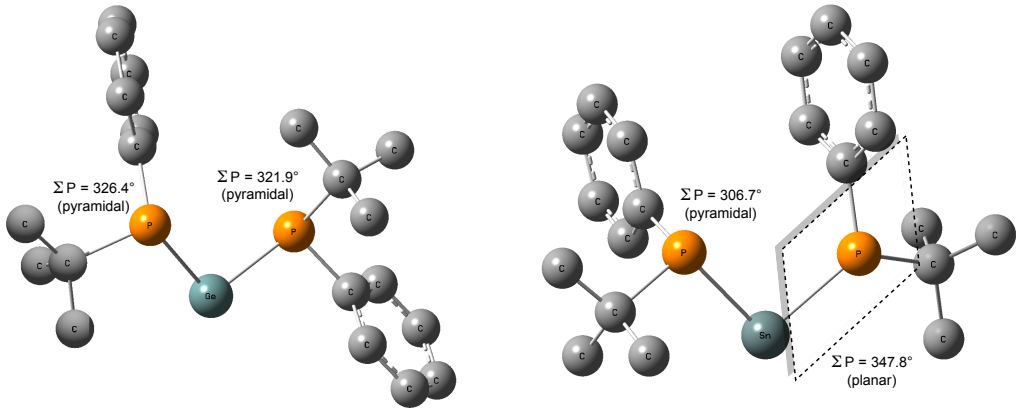


Figure 2.3.: mPW1PW91/SDD DFT calculated global minima for $(PhP^tBu)_2Ge$ and $(PhP^tBu)_2Sn$ showing the pyramidalisation of the P centres

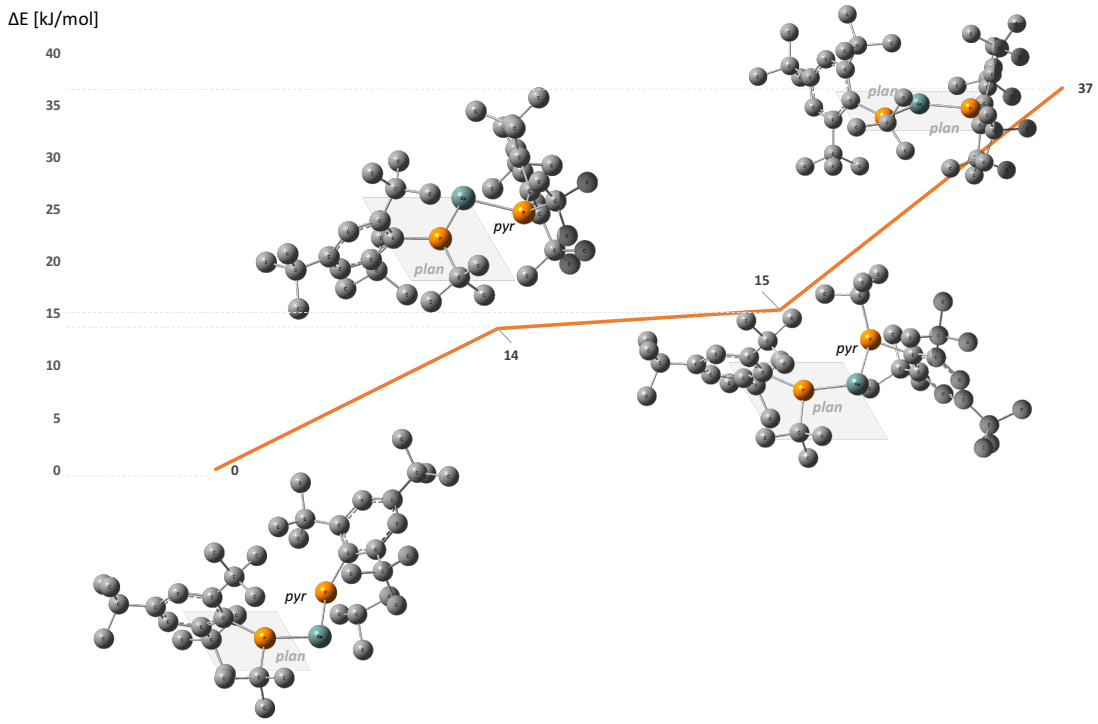


Figure 2.4.: mPW1PW91/SDD DFT calculated structures for $(Mes^*P^tBu)_2Ge$ showing 4 conformers and their relative energies

In the tin congener, (Mes*P^{t}Bu)$_2$Sn, the global minimum is 15 kJ/mol more stable than the other minima. The Sn-P distances are 2.52$\AA$ and 2.71$\AA$, with a P-Sn-P angle of 104.2°. The bond angle sums of the P atoms are 360° and 325°, respectively.

Looking at the **TMS** substituted compound, (Mes*PTMS)$_2$Ge, there were 4 minimum structures detected, from which only one has a planar phosphorus centre. Again this is the least stable conformer. The global minimum is a very symmetric compound with similar P-Si/P'-Si and P-Ge/P'-Ge values (see Table 2.1). For the TMS substituted stannylenes, (Mes*PTMS)$_2$Sn, bond angle sums of 347.0° and 360.0° were detected. The P-Sn-P angle is with a value of 110.3°, slightly wider. Interestingly, as seen in the above discussed phenyl substituted compound, a conformer with two almost planar P atoms, $\sum$ P(P)' = 355.6° (355.0°), was found. Again, this conformer was the least stable one, with an $\triangle$H of 20 kJ/mol.
With the sterically demanding Hyp group substituted compounds show an increased P-Sn-P' angle, due to the ligand size, which can be seen in Table 2.3. Again more than one conformer could be detected, from which the global minimum has a planar and a pyramidal centre. We can see a shorter bond to the planar centre together with an elongation of the second P-Sn bond.

Using the bulky Hyp group, forming **(HypPR)$_2$E**, the global minima of those compounds have usually two pyramidal phosphorus centres. As mentioned before, NBO analyses show in these cases interactions between the P lone pairs with the empty p orbital on E (= Ge, Sn) with lower delocalisation energies (E_2 = 15 - 30 kcal/mol) than in compounds with planar P centres.
For (Hyp^{t}BuP)$_2$Ge, (Hyp^{t}BuP)$_2$Sn and (Hyp$_2$P)$_2$Sn global minimum structures with one planar P centre were detected. In these cases we see higher delocalisation energies, simultaneously the bond from the pyramidal P centre to the group 14 element gets significantly elongated, which weakens the molecule.
For the germylenes substituted with **^{t}Bu**, (Hyp^{t}BuP)$_2$Ge, only one stable conformer could be determined. It is a compound with one pyramidal and one planar P centre, and an P-Ge-P' angle of 103.0 °.
For the **TMS** substituted compound, (HypTMSP)$_2$Ge, only one conformer was

detected, this compound has two pyramidal centres and is symmetric with an P-Si/P'-Si bond length of 2.35 $\AA$ and an P-Sn/P-Sn bond length of 2.41 $\AA$. For the **^{t}Bu** substituted stannylenes, (Hyp^{t}BuP)$_2$Sn, all of the minima are rather close in energy (ΔH = 3.1 - 16.5 kJ/mol). The global minimum has Sn-P distances of 2.51$\AA$ and 2.69$\AA$ and the P bond angle sums are 360° and 309.7°.
For the analogous compound with **TMS**, (HypTMSP)$_2$Sn four minima were found only 1.7 to 3.4 kJ/mol less stable than the global minimum and another four minima were located with ΔH = 8.8 kJ/mol to 24.8 kJ/mol. The global minimum is quite symmetric, both Sn-P distances are 2.59$\AA$ and both P atoms are pyramidal with a bond angle sum of 328°.
All calculated minimum structures (coordinates and E) are given in the appendix.

Calculating the corresponding ^{31}P NMR shifts can be a great benefit for the synthetic approach. Especially for the germylenes this can be an advantage, because there is less data known in literature and ^{73}Ge NMR data is scarcely accessible. DFT calculations for ^{31}P NMR shifts can serve as guideline values for the experiment. Because of the HALA (Heavy Atom on the Light Atom) effect, a general deshielding of ^{31}P NMR shifts of P attached to a heavy atoms (Ge, Sn) is expected.
Concerning the NMR data of our calculated compounds, two shifts in the ^{31}P NMR should be detected if a conformer has one pyramidal and one planar P centre. In the germylenes, ^{31}P shifts for compounds with two pyramial P centres, can be detected in a range of 80 - 160 ppm. In conformations with a planar and a pyramidal P centre, we expect down field shift around 100-170 ppm and a high field shift at -16 - 1.5 ppm. A diphosphagermylene, (PDipp$_2$)$_2$Ge, isolated by Izod,[79] shows ^{31}P CP-MAS solid-state NMR peaks at 81.9 ppm and -61.6 ppm in a 1:1 ratio. This experimental approach was supported by DFT calculations, which predicted chemical shifts for the planar and pyramidal phosphorus for 100 and -61 ppm.[79]

This is consistent with our calculations, since our comparable compounds, (PhPHyp)$_2$Ge and (Mes*PHyp)$_2$Ge, show ^{31}P NMR values of 98.12/-16.44 ppm and 115.2/-16.22. Since we have a silyl ligand on the P atom, the signals

differ slightly from Izod's calculations for two aromatic carbon ligands on the P centres. The electronegativity of the substituents and the changing bond angle on the phosphorus atom have the strongest influence on the chemical shift. As already stated in literature there is no linear or constant change with increasing degree of substitution.[80] The ^{31}P shifts can however be qualitatively explained with the electronegativity of the neighbouring atoms of the phosphorus atom and the bond angle. Sterically demanding substituents, such as ^{t}Bu, rather produce a downfield shift that the less bulky Me or Ph group.[80]

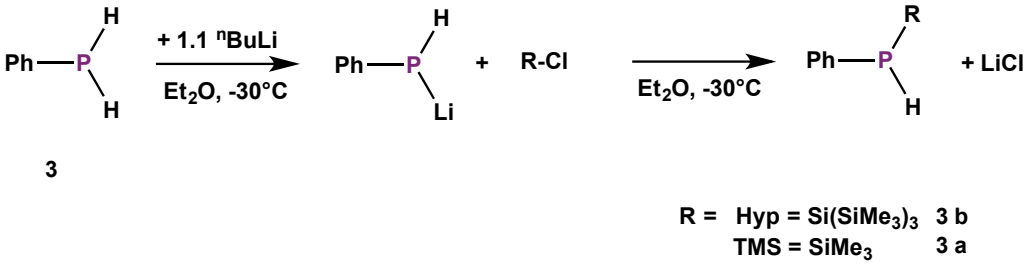
Table 2.4.: mPW1PW91/Iglo-II DFT calculated NMR data for heteroleptic tetrylenes

Compound	^{31}P [ppm]	^{29}Si [ppm]	^{73}Ge [ppm]	^{119}Sn [ppm]
(PhPR)$_2$Ge				
Substituent R				
^{t}Bu	161/147		1203	
TMS	87/83	24/23	1389	
Hyp	98/-16	-3/-6/-49/-51	1090	
(PhPR)$_2$Sn				
^{t}Bu	118/95			1509
TMS	20/16	22/24		1793
Hyp	38/-87	-2/-3/-5/-8-52		1298
(Mes*PR)$_2$Ge				
Substituent R				
^{t}Bu	178/1.5		479	
TMS	66/32	19/18	478	
Hyp	115/-16	-2/-3/-7/-40/-47	1329	
(Mes*PR)$_2$Sn				
^{t}Bu	181/-2.3			591
TMS	61/18	20/17		563.22
Hyp				
(HypPR)$_2$Ge				
Substituent R				
^{t}Bu	177/-6	13/-3/-4/-58/-78	744	
TMS	3	14/-1/-6/-17	1296	
(HypPR)$_2$Sn				
^{t}Bu				
TMS	22/-139	14/-1/-2/-4/-5/-62/-68		1338

The shifts for the planar phosphorus atom are calculated to occur in our investigated stannylenes in a region from 22 to 52 ppm, while the pyramidal phosphorus centres resonate in the highfield from -139 to -125 ppm. In literature known compounds isolated by Izod[49] with molecular formula $(R_2P)_2Sn$ [R

= Dipp (2,6-$^{i}Pr_2C_6H_3$) or Tripp (2,4,6-$^{i}Pr_2C_6H_3$)] show ^{31}P NMR peaks at -25.1 ppm with a P-Sn coupling of 1300 Hz and -19.5 ppm with a P-Sn coupling of 1420 Hz in a toluene-d_8 solution. Intriguingly, there was only one signal detected, although the compound was stated to have two different P centres, a planar and a pyramidal one, seen in the corresponding crystal structures. While in the solid-state $^{31}P(^{1}H)$ MAS NMR spectra of the Dipp substituted compound, shifts at 95.8 ppm (P-Sn = 2620 Hz) and -66.2 ppm (P-Sn = 1180 Hz) occurred,[49] which matches their DFT calculations, predicting chemical shifts for the planar and pyramidal P centres at 94 and -67 ppm.[49] Izod[49] mentioned low energy barriers for his compounds. There is a high possibility of an equilibrium of both conformers in solution. Thus they could only detect one signal, which is in the expected region for pyramidal P atoms.

As mentioned before, tetrylenes are interesting candidates for complementing transition metal compounds in catalytic processes. Particularly the activation of small molecules, such as H_2 and NH_3, arouses great interest. Schoeller[81] noted that HOMO-LUMO gaps, $\Delta_{H\text{-}L}$, and singlet-triplet energy separations, $\Delta_{S\text{-}T}$, are essential in the reactions with small molecules. Smaller gaps lead to lower activation barriers and are therefore favourable.[49] Recently, it was mentioned[82] that by the use of phosphido ligands, the values for $\Delta_{S\text{-}T}$ can be lowered to values below 63 kJ·mol^{-1}. In diaminotetrylenes, the values are around 88 kJ·mol^{-1} or higher. Literature known germylenes,[83] which were tested for H_2 activation show HOMO-LUMO gap values from 3.4-3.6 eV. Comparing with our results, we can see that in all Sn conformers seen in Table 2.2, the HOMO-LUMO energy gaps are between 2.04 eV and 3.25 eV. If we take a closer look at our TMS substituted compounds, (Mes*PTMS)$_2$Sn and (HypPTMS$_2$)Sn, the absorption maximum for the Mes* compound is at 531 nm (red-purple) and the absorption maximum for the Hyp compound is at 676 nm (green blue). This indicates a smaller HOMO-LUMO gap for the (HypPTMS$_2$)Sn, which could be confirmed with our DFT calculation; the $\Delta_{H\text{-}L}$ value for the Hyp compound is 3.11 eV, while the Mes* compound has a wider gap of 3.25 eV. The $\Delta E_{S\text{-}T}$ could be calculated with 128.5 kJ·mol^{-1} for (Mes*PTMS)$_2$Sn and 178.7 kJ·mol^{-1} for (HypPTMS)$_2$Sn. This makes these compounds ideal candidates for the activation of small molecules.



Scheme 2.1: Reaction route to $PhPHR_2$ with R = TMS or Hyp

All three investigated backbone systems (Ph, Mes*, Hyp) together with the ligands ^{t}Bu, TMS or Hyp were considered for DFT calculations on diphosphatetrylenes. In sum, the Mes* and Hyp backbone in combination with a ^{t}Bu or TMS ligand seem to provide enough steric stabilisation for the isolation of monomeric diphosphatetrylenes.

2.2. Synthesis and characterisation

Using the calculated results the experimental approach focused on various phosphanes and phosphanides, that could act as ligands for low valent group 14 compounds.

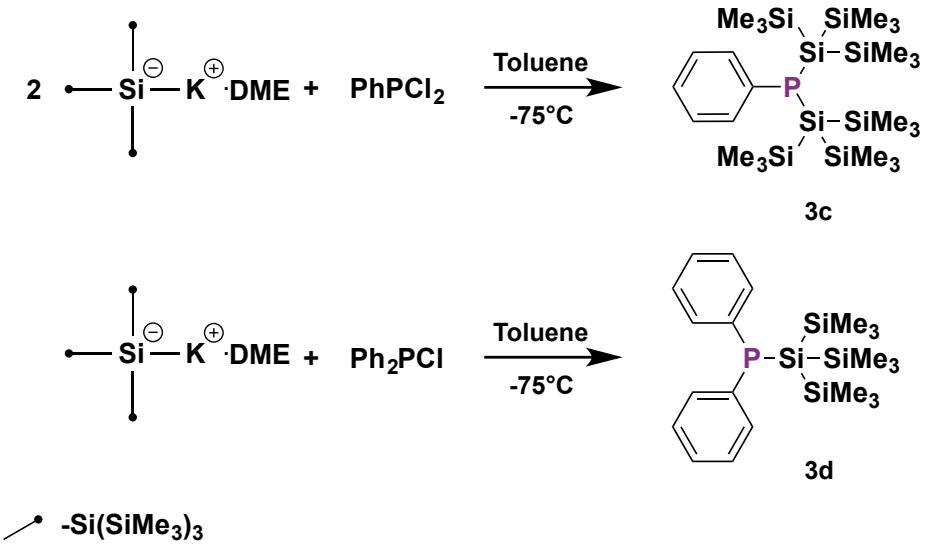
2.2.1. Phenylsilylphosphanes

$PhPH_2$ is a quite small and highly reactive molecule, which is pyrophoric, once exposed to atmosphere. The synthesis of PhTMSPH ($C_6H_5PH(SiMe_3)$) was reported before,[84,85] however previous mentioned methods use either alkali phenylphosphasilanes or the reaction of diarylphosphanes or diaminophosphanes with lithium and chlorosilanes for the formation of the desired product. In another method primary or secondary phosphanes were reacted with organo halides in the presence of Schwesinger bases,[86] which led to high yields. We used a more direct pathway (see scm.2.1), a lithiation of $PhPH_2$ with ^{n}BuLi, followed by a salt elimination reaction with TMS-Cl. **3a** is highly reactive and tough to isolate under ambient conditions. The compound was characterised via NMR (^{31}P = - 133.2 ppm, $^{1}J_{P\text{-}H}$= 210 HZ).

Instead we moved on to a bulkier chlorosilane, Hyp-Cl. Similar to the previous reaction pathway, lithiation of $PhPH_2$ **3** with ^{n}BuLi is follwed by a salt elimination reaction with hypersilylchlorosilane. This reaction pathway and the conversion with Hyp-Cl was not reported before. Compound (PhHyp)P-H, **3b**, could be isolated as an colourless oil and was characterised via NMR. A ^{31}P NMR chemical shift of -132.9 ppm fits to a primary silylphosphane. ^{29}Si NMR peaks were found at -10.35 ppm ppm for the (-Si(**Si**$Me_3)_3$) with an $^{2}J_{Si\text{-}P}$ coupling constant of 9 Hz and a peak at -94.82 ppm for (-**Si**$(SiMe_3)_3$) with and $^{1}J_{Si\text{-}P}$ coupling constant of 86.0 Hz, similar to the before discussed PhTMSPH **3a**. The calculations give a ^{31}P shift of -117.4 ppm, which is in an adequate range for calculated phosphorus shifts (see Table 2.3).

As mentioned before, especially the bulky hypersilyl group ($Si(SiMe_3)_3$) can be beneficial in terms of stabilising silylphosphanes and further for the synthesis of low valent main group compounds. Due to calculations a compound of type $PHyp_3$ should have an $\sum$ P(P)' = 341.7°, which is almost planar. However, this compound is unstable. There are highly reactive ·$SnHyp_3$ and ·$PbHyp_3$ radicals known, where crystal structures of the corresponding alkali metal tetrelanides ((($Et_2O)_2KPbHyp_3$) and $(Et_2O)_2KPbHyp_3$)) could be isolated when storing inert at -65°C.[87] The yields of the homoleptic tetryl radicals are far from quantitative, several diamagnetic compounds could be detected as side-products by NMR spectroscopy.[87]
Compounds of type $PhPHyp_2$ and Ph_2PHyp, which are more likely synthetic feasible, result in smaller angle sums of 324.7° and 312.1° (see Table 2.1), but have a higher ability to shield the active centre E due to bulkiness.

The doubly Hyp silylated phosphane, Hyp_2Ph, could neither be isolated via the direct nor the stepwise reaction pathway shown in scm. 2.2. The stepwise reaction pathway to form Ph_2PHyp was successful and a novel diphenylsilylphosphane could be isolated in good yields (see fig.2.5). Despite the compound featuring high reactivity, it could be isolated in solid state. A comparison of calculated and experimental data can be found in Table 2.5.



Scheme 2.2: Reaction of chlorophenylphospanes with potassiumhypersilanide

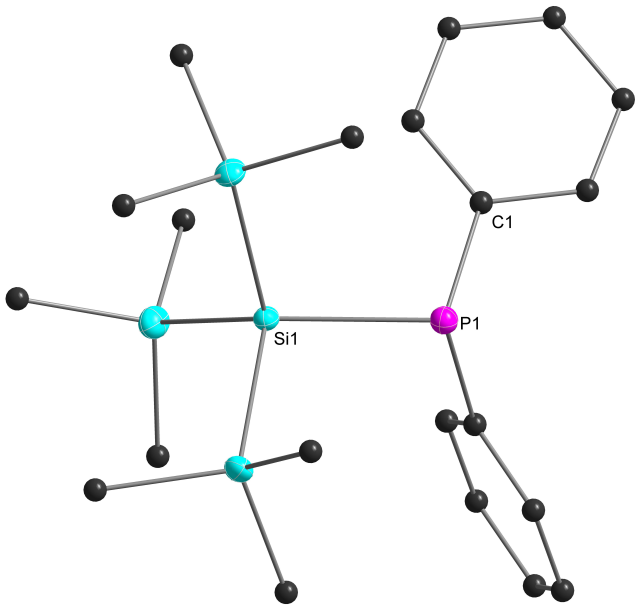


Figure 2.5.: Ph_2PHyp **3d**. Hydrogen atoms have been omitted for clarity

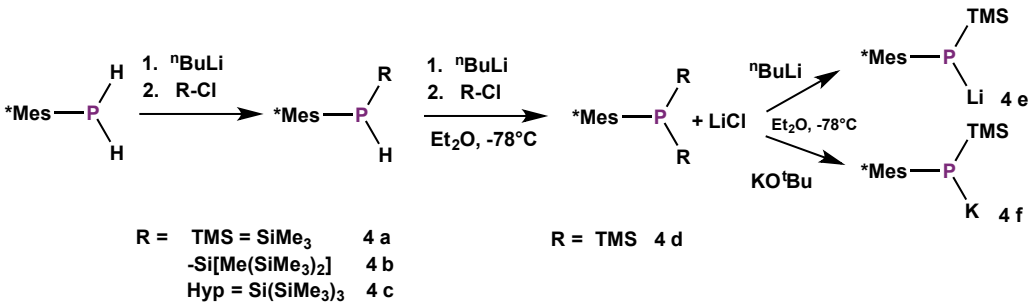
Table 2.5.: mPW1PW91/SDD DFT calculated and experimental data for the Ph_2PHyp **3d**

Bond lengths	exp. [$\AA$]	calc. [$\AA$]
P1-Si1	2.28	2.33
P1-C1	1.84	1.86
P1-C7	1.84	1.85
Si1-Si2	2.37	2.41
Si1-Si3	2.35	2.41
Si1-Si4	2.36	2.40
Bond angles [°]	exp. [°]	calc. [°]
C-P-C	101.2	103.2
Si-P-C1	107.2	108.7
Si-P-C7	106.3	107.1
$\Sigma\alpha$(P) [°]	314.7	312.1
^{31}P NMR [ppm]	$\delta_{exp.}$	$\delta_{calc.}$
	δ-49.76	δ -23.5
	($^1J_{P\text{-}Si}$= 73 Hz; $^3J_{H\text{-}P}$= 6.5Hz)	
^{29}Si NMR [ppm]	δ -88.9	δ -94.5
	δ ($^1J_{Si\text{-}P}$ = 76 Hz)	
	δ -9.74	δ -26.6
	δ ($^2J_{Si\text{-}P}$ = 12 Hz)	

2.2.2. Supermesitylsilylphosphanes and -phosphanides

The next investigated system is Mes*PH_2, **4**, where the hydrogens were replaced by a variety of silyl ligands (see fig.2.3), beginning with the commonly used TMS group. The lithiation of Mes*PH_2 with ^{n}BuLi is well known and yields the phosphanide Mes*PHLi. Straightforward salt elimination reaction with TMS-Cl yields the silylphosphane Mes*P(TMS)H . This phosphane was first mentioned in the early 1980s,[88] where it was used in the synthesis of diphosphenes. A subsequent reaction with ^{n}BuLi and a salt elimination reaction with TMS-Cl leads to Mes*$P(TMS)_2$. The deprotonation reaction with ^{n}BuLi can also yield the diphosphene. The Mes* substituent can protect the unstable P=P bond as has been shown before.[89]

However, both compounds (Mes*TMS)PH and Mes*$PTMS_2$ could be characterised via NMR and were further used for synthesis. Mes*PTMSH shows a ^{31}P peak at -128.9 ppm and a $^1J_{P\text{-}H}$ coupling of 212.0 Hz could be detected, consistent with literature data[90] and calculated data (^{31}P = -112.8 ppm).^{29}Si data



Scheme 2.3: Reaction route to supermesityl phosphanes and phosphanides

was not reported to date. We could detect a shift at 8.85 ppm, with an $^{1}J_{Si\text{-}P}$ coupling constant of 21.2 Hz. In the case of Mes*PTMS$_2$, **4d**, no P-H coupling could be detected, confirming complete conversion of the educt. The ^{31}P peak of **4d** is shifted to -146.0 ppm and ^{29}Si satellites were observed (see fig. 2.7). The ^{29}Si shift is a doubletic triplet at 5.5 ppm, this compound can be compared to $C_6H_4(P(SiMe_3)_2)_2$-1,2. This compound shows a sharp ^{31}P peak at -140.4 ppm and ^{29}Si shift at 2.56 ppm, also a dupletic triplett. The X-ray structure of compound $C_6H_4(P(SiMe_3)_2)_2$-1,2 can be seen in fig.2.6 and the corresponding NMR data of Mes*PTMS$_2$ and $C_6H_4(P(SiMe_3)_2)_2$-1,2 in fig.2.7.

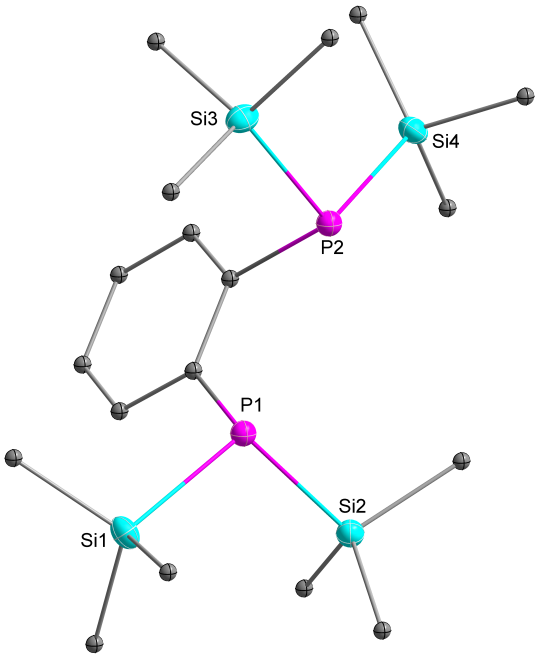


Figure 2.6.: Structure of $C_6H_4(P(SiMe_3)_2)_2$-1,2 obtained by X-ray diffraction analysis. Hydrogen atoms have been omitted for clarity

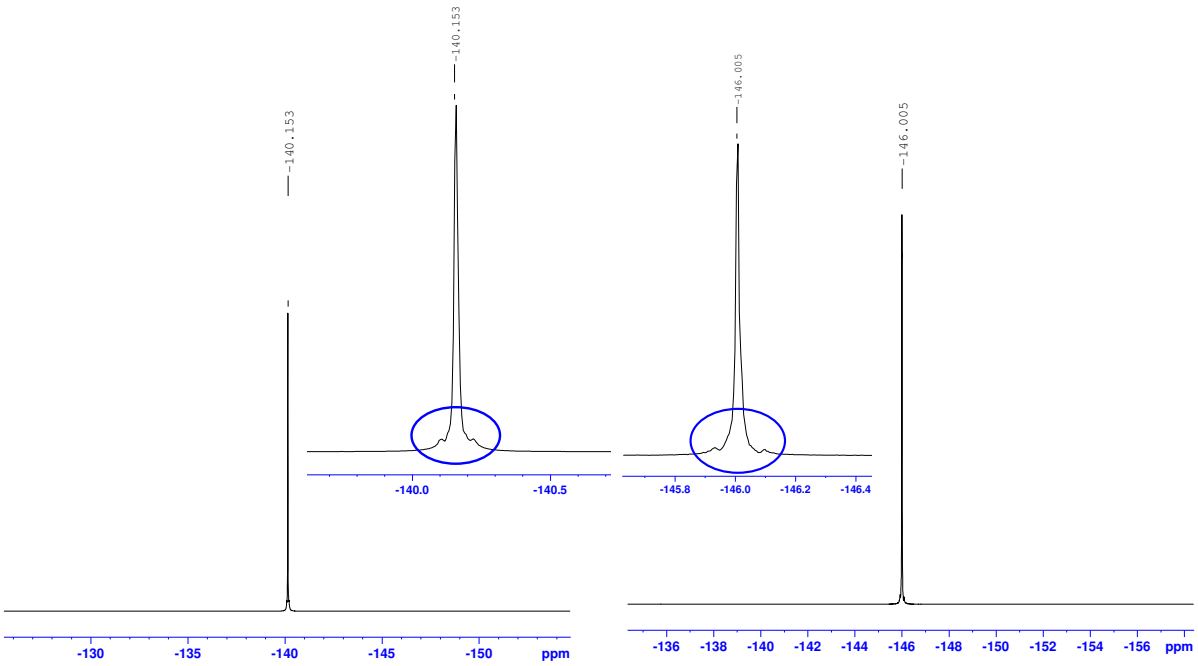


Figure 2.7.: Comparison of ^{31}P NMR data of $C_6H_4(P(SiMe_3)_2$ (left) and compound **4d**

Reaction of **4d** with ^{n}BuLi causes an almost quantitative (99%) abstraction of one trimethylsilyl group, resulting in the clean isolation of lithium phosphanide **4e**. Si-P cleavage by KO^{t}Bu or ^{n}BuLi, as well as lithiation of primary and secondary phosphanes, is a well known reaction. However, solid state structures of **4e** and **4f** were not reported to date. Crystals suitable for X-ray diffraction analysis were gained from a mixture of n-hexane and toluene (see fig.2.8 and 2.9). A P-C bond length was observed with a length of 1.872 $\mathring{A}$ for the lithium phosphanide **4e** and 1.887$\mathring{A}$ for the potassium phosphanide **4f**, the values for the P-Si bond (2.226 $\mathring{A}$ and 2.211 $\mathring{A}$) are in a reasonable region. Both phosphanides crystallize as dimers consisting of two metal atoms bridged by two Mes*P- ligands in a P-M-P-M central ring (M = Li, K). In the case of **4e**, one Li coordination centre is saturated by ether, while the second Li atom is stabilised by agostic interactions from the t-butyl groups of the Mes* ligand, with a coordination number of 2. The values for these Li···H-C contacts are within reported values for a Li···H-C (2.140 $\mathring{A}$, 2.365 $\mathring{A}$ and 2.745 $\mathring{A}$) agostic interaction.[91] The P-Li bonds are with 2.505 $\mathring{A}$ and 2.412 $\mathring{A}$, comparable to the literature known lithium phosphanide [LiPMes$_2$)(OEt$_2$)]2,[15] with P-Li bonds of 2.483 $\mathring{A}$ and 2.479 $\mathring{A}$. In case of the potassium phosphanide **4f**, each metal atom is coordinated to DME. The K···H-C contacts are as well within reported

values for a K···H-C (2.845 $\mathring{A}$, 3.062 $\mathring{A}$, 3.101 $\mathring{A}$ 3.238 $\mathring{A}$) agostic interaction.

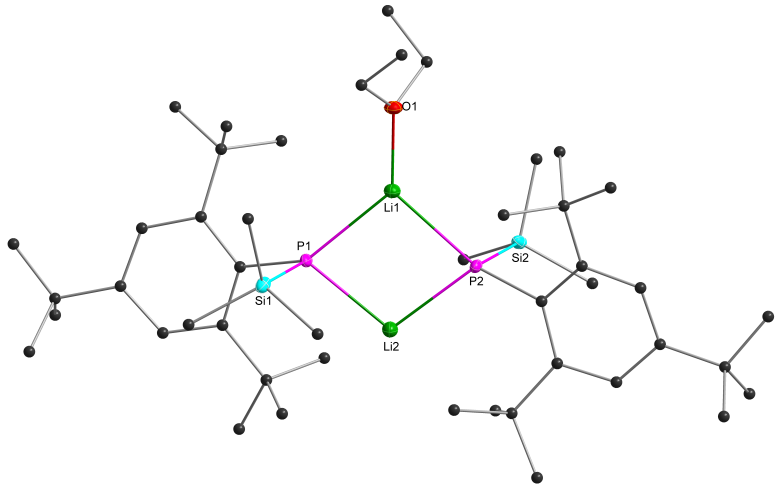


Figure 2.8.: 2,4,6-tris(*t*-butyl)phenyl trimethylsilyl-lithium-phosphanide **4e** obtained by X-ray diffraction analysis. Hydrogen atoms have been omitted for clarity.

To avoid the deprotonation reaction and the dimerisation to Mes*P=PMes* (fig. 2.10), a change of the silyl substituent to a more sterically demanding one was done. The probability of formation of P=P double bonds decreases and pure monomeric silylphosphanes become accessible. Introducing the -Si[Me($SiMe_3$)$_2$] group resulted in the isolation of a novel silylphosphane, **4b** (see fig.2.11). Starting from Mes*PH_2, and lithiation with ^{n}BuLi, the compound could be isolated after a salt elimination reaction with Cl-Si[Me($SiMe_3$)$_2$]. The compound is air sensitive, as other similar phosphanes,[90] Crystals suitable for X-ray analysis could be obtained. The compound was characterised *via* NMR. This novel silylphosphane has a sharp ^{31}P peak at -127.2 ppm, with an $^1J_{P\text{-}H}$ coupling constant of 221.8 Hz. In this case more than one silicon shift is expected, the ^{29}Si shift for -Si[Me(**Si**Me_3) occurs at 7.40 ppm, with an $^2J_{Si\text{-}P}$ coupling constant of 17.5 Hz. The -**Si**[Me($SiMe_3$)$_2$] occurs at -50.62 with an $^1J_{Si\text{-}P}$ coupling constant of 71.0 Hz.

In order to further increase the steric bulk, an even bulkier silyl group, Hyp, was used. In this case a novel silylphosphane could be isolated (see fig. 2.12). Again starting from Mes*PH_2, and lithiation with ^{n}BuLi, the compound could be

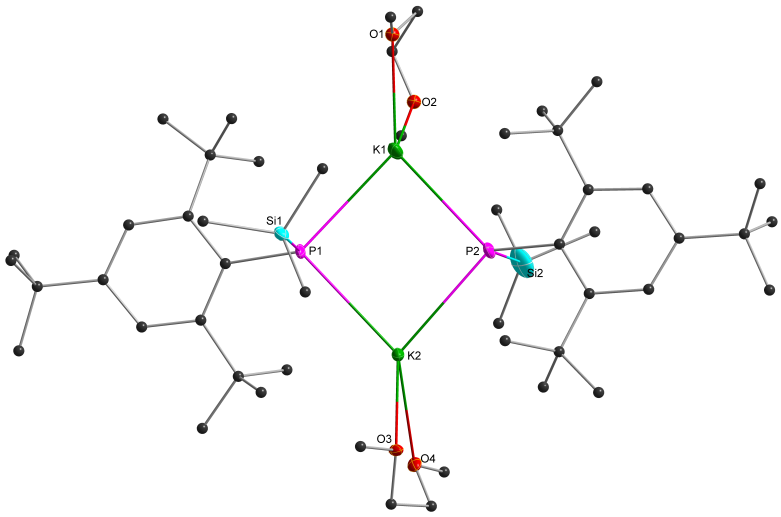


Figure 2.9.: Structure of 2,4,6-tris(*t*-butyl)phenyl trimethylsilyl potassium phosphanide]·DME **4f** obtained by X-ray diffraction analysis.

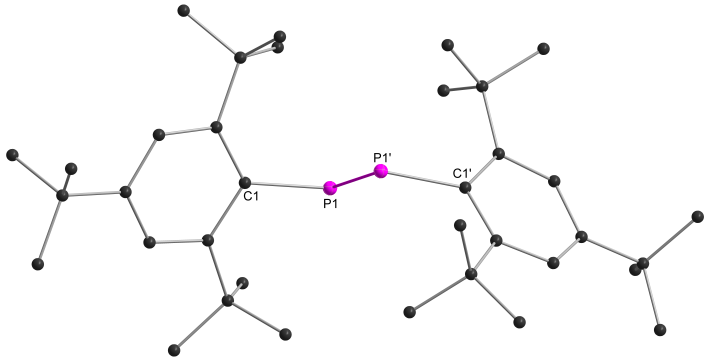


Figure 2.10.: Structure of 1,2-bis[2,4,6-tris(1,1-dimethylethyl)phenyl]-diphosphene . Hydrogen atoms have been omitted for clarity.

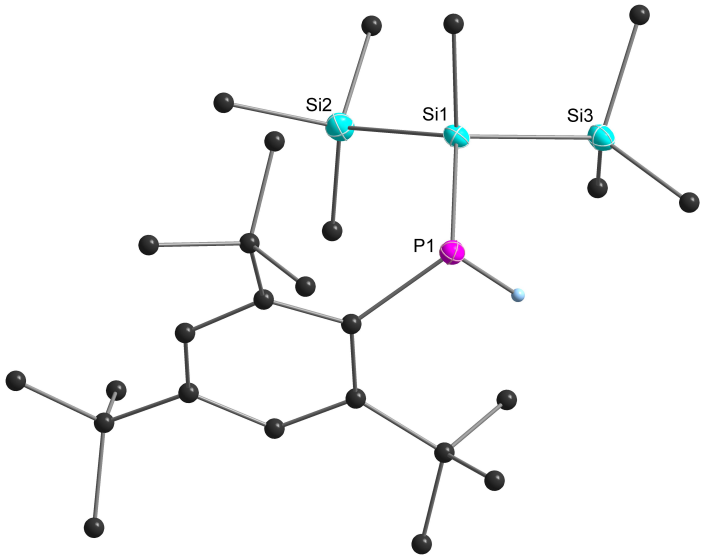


Figure 2.11.: (Si[Me(SiMe$_3$)$_2$]Mes*)P-H **4b** obtained by X-ray diffraction analysis. Hydrogen atoms have been omitted for clarity

isolated after a salt elimination reaction with Hyp-Cl. Again the silylphosphane is highly reactive towards air and moisture. A ^{31}P peak was detected at - 137.8 ppm with an corresponding $^{1}J_{P\text{-}H}$ coupling constant of 220.6 Hz. ^{29}Si shifts were detected -83.0 ppm -**Si**(SiMe$_3$)$_2$, and -9.5 ppm -Si(**Si**Me$_3$)$_2$. The corresponding coupling constants are $^{1}J_{Si\text{-}P}$ = 67.5 and $^{2}J_{Si\text{-}P}$ = 5.62 Hz. The experimental data (-137.8 ppm) is in agreement with the calculated ^{31}P value of -146.1 ppm. The calculated bond lengths and angles are congruent to the experimental data (see Table 2.6).

NMR data of all compounds can be compared to the DFT calculated data, see Table 2.6.

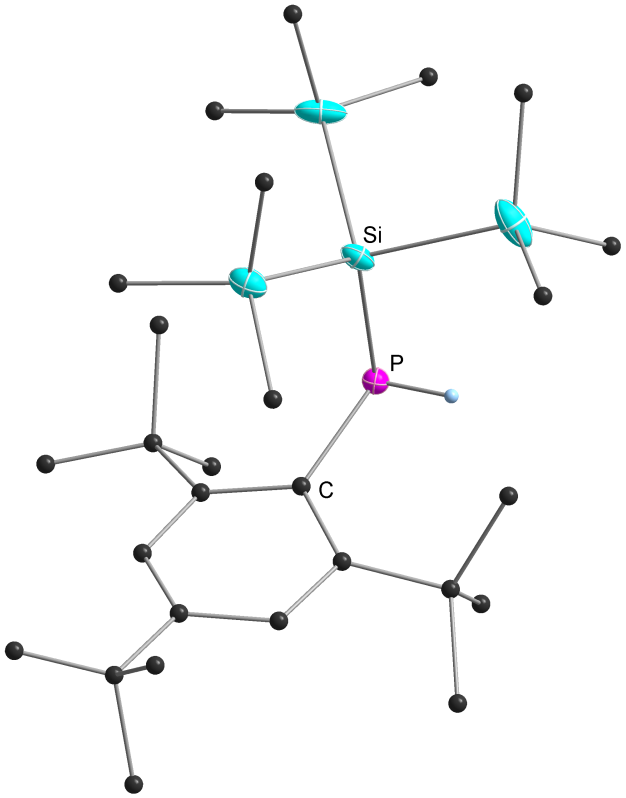


Figure 2.12.: (HypMes*)P-H **4c** obtained by X-ray diffraction analysis. Hydrogen atoms have been omitted for clarity

Table 2.6.: DFT calculated and experimental ^{31}P NMR data for silylphosphanes

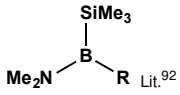
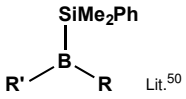
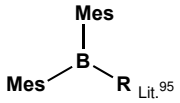
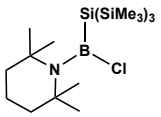
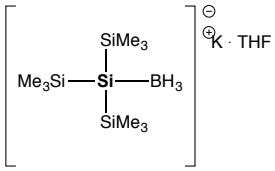
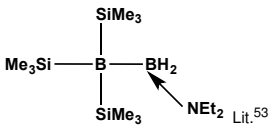
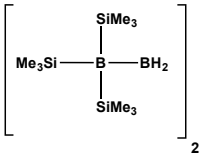
compound	δ $^{31}P_{exp.}$	$^{31}P_{calc.}$
$PhPH_2$	-125.5	-122.8
Ph_2PH	-55.5	-35.8
PhPTMSH	-133.2	-146.1
PhPHypH	-132.9	-117.4
$PhPHyp_2$	-137.3	-180.6
Ph_2PHyp	-57.00	-23.5
Mes^*PH_2	-131.4	-153.9
$Mes^*P(TMS)H$	-128.9	-112.8
$Mes^*P(Si(SiMe_3)_2Me)H$	-127.2	-138.1
$Mes^*P(Hyp)H$	-137.8	-146.1
Mes^*PTMS_2	-146.0	131.2
DBP(TMS)$_2$ $C_6H_4(P(SiMe_3)_2)_2$-1,2	-138.7	-105.4
$HypP(TMS)_2$	-268.8	-221.2
$HypP^tBu_2$	-	57.10

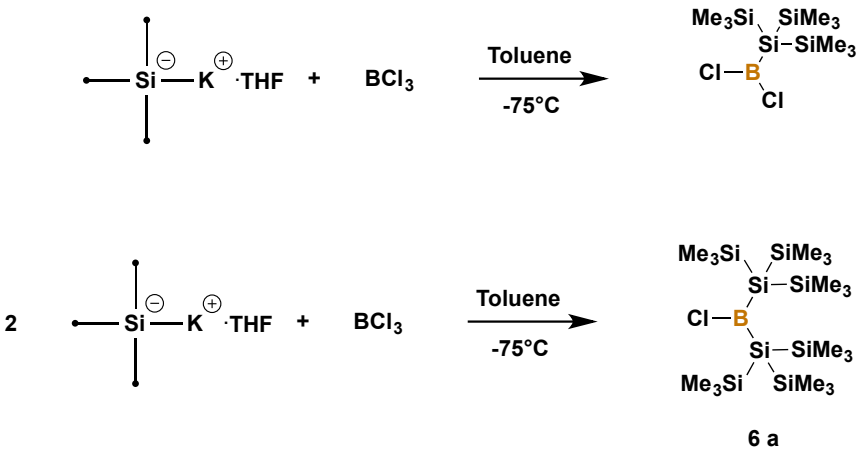
2.3. Open and cyclic double silylated boron compounds - chasing trisilylboranes

The activation of small molecules is a heavily discussed topic in modern organometallic chemistry. Apart from transition metal complexes, main group compounds were found to feature great reactivity towards small molecule activation. Recently, calculations showed that disilylboranes should be able to activate H_2.[51] Stabilisation of η^2-H_2 complexes can be provided via donation to the empty orbital of the boron and backdonation from the B-R orbitals, which seems to work especially well for silyl ligands such as TMS (-Si(Me)$_3$) or Hyp (-Si(SiMe$_3$)$_3$). This donation/backdonation "mechanism" is comparable to carbenes or their heavier congeners. The amount of publications containing silylboranes is still quite small, although first substances containing silicon boron bonds were reported in the 1960s.[92] In the last decade, the interest in silylated boron compounds increased due to the various catalytic possibilities in metallorganic chemistry.
Just recently first silyl- and germylboryl complexes were obtained *via* (dichloro)silyl- and (dichloro)germylboranes.[93] Silyl(mono)boranes are in general produced via a reaction of silyl anions with boron halides. A common side reaction is the formation of tetracoordinated borate, thus the boron has to be either sterically or electronically shielded. In most compounds containing Si-B bonds, stabilisation can be provided *via* amino groups (Me_2N, Et_2N), or adding those amino groups as auxiliary bases. Otherwise stabilisation is provided with bulky aryl substituents, such as Mes (1,3,5-trimethylbenzene). An overview of literature known silylboranes and corresponding NMR data can be found in Table 2.7.

As before mentioned, the reaction of hypersilyl anions with chlorophosphanes is a neat way for synthesising novel silylphosphanes. Therefore, the very versatile tris(trimethylsilyl)silyl group (Hyp) was chosen for research on silylboranes. Various reaction pathways for the isolation of stable linear and cyclic silylated boranes were explored (see scm.2.4, 2.5 and 2.6). Since the formation of trisilylboranes was the desired task, a formation of a cycloborosilane is an interesting possibility (see scm. 2.6). A similar reaction pathway was introduced by Markov[52] in 2004 (see fig.2.15). Reaction with boron halides

Table 2.7.: ^{11}B and ^{29}Si NMR data of some literature known silylboranes

compound	R / R'	$\delta\ ^{11}B_{lit.}$	$^{29}Si_{lit.}$
 Lit.[92]	Cl	41.3	
	OCH_3	33.8	
	O^tBu	32.2	
	SCH_3	46.9	
 Lit.[50]	NEt_2 / NEt_2	36.5	
	NEt_2 / Cl	40.7	
	NEt_2 / Me	49.1	
	NEt_2 / ^tBu	50.0	
	NEt_2 / $SiMe_2Ph$	55.7	
	N^iPr_2 / N^iPr_2	41.2 Lit.[94]	
 Lit.[95]	$SiPh_3$	101	-28.6
	$SiPh_2BDMA$ (= Dimethylbenzylamine)	102	-30.2
	$SiPh_2Mes$	101	-28.4
 Lit.[52]		48.5	-10.9
 Lit.[53]		-43.3 q, J_{B-H} = 84 Hz	-10, -125.5 q, J_{Si-B} = 51 Hz
 Lit.[53]		-12.7 q, J_{B-H} = 105 Hz	-9.8 q, J_{Si-B} = 51 Hz
 Lit.[53]		34.3 (broad)	-10.5

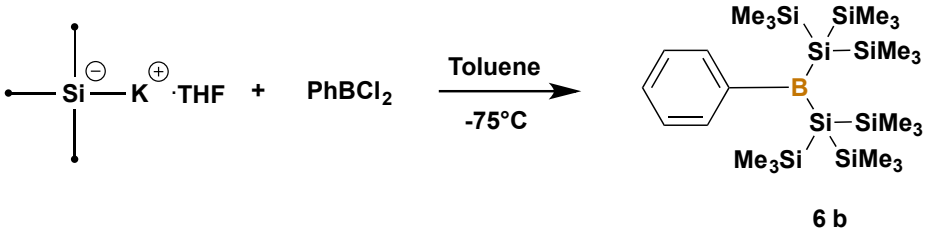


Scheme 2.4: Pathway 1 of boron trichloride with potassiumhypersilanide

should give an chlorosilylborolane, providing a boron surrounded with two silicon atoms, and an additional Cl functionality, which could be further reacted with an anionic silyl group (e.g. Hyp-K).

At first a reaction pathway similar as for our isolated silylphosphanes was pursued. For the boron compounds, hypersilylpotassium has to be prepared in THF rather than DME, because boron halides react with DME and form boraxanes (see fig.2.13 and 2.14). Switching back to THF goes along with longer reaction times, up to 24 h. However, heating up the reaction to 55°C enabled full conversion to HypK after 2 h reaction time.

Pathway 1 with BCl_3 led to the isolation of slightly grey-green oils. The reaction was performed in a 1:1 and 2:1 ratio (HypK : BCl_3) to possibly form mono or disilylboranes. Equal quantities of educt result in a product mixture of the desired product $HypBCl_2$, $Hyp_2BOSiMe_3$ and HypH. The calculated ^{11}B NMR shift for $HypBCl_2$ is at 83.2 ppm with a coupling constant of 81 Hz (see Table 2.8). In the experimental data a small ^{11}B shift at 82 ppm could be detected, the main peak was still BCl_3, which encouraged the excess use of HypK. The GC-MS data confirmed the formation of $Hyp_2BOSiMe_3$ (M^+ = 593) and HypH (M^+ = 248). The main peak however was detected with M^+ of 255, which fits to HypBR, a mixture of $HypBCl_2$ and Hyp_2BCl. This mixture can't be separated properly.
Using 2 equivalents of HypK led to an increased peak at 82 ppm, and total



6 b

Scheme 2.5: Pathway 2 of dichlorophenylborane with potassiumhypersilanide

conversion of the silyl anion. The GC-MS data again revealed a product mixture of $Hyp_2BOSiMe_3$, HypR and Hyp_2BR with an M^+ of 669, which is more likely to be attributed to $HypBCl_2$.

This reaction pathway was not as successful, due to the high reactivity of BCl_3. A change to a more stable and sterically demanding borane, $PhBCl_2$ (see scm. 2.5). With the use of $PhBCl_2$, the formation of Hyp_2BPh could be confirmed via NMR and GC-MS. The slightly green oil was stored at -30°C in order to gain crystals from this viscous solution. The ^{11}B of this solution gave a peak at 63.5 ppm. This does not fit to calculated data (see Table 2.8), but the GC-MS data showed the formation of the desired product with an M^+ of 583, together with the side products $HSi(SiMe_3)_3$ (M^+ = 247) and $ClSi(SiMe_3)_3$ (M^+ = 282). The NMR analysis revealed unreacted educt, therefore an excess use of HypK should be tried.

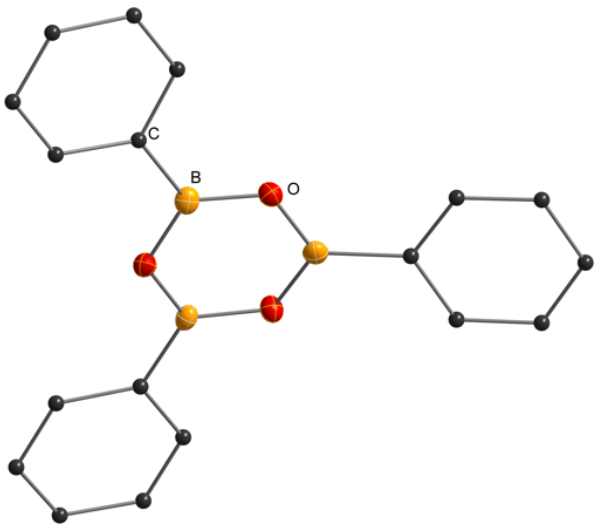


Figure 2.13.: Reaction product of hypersilylpotassium and dichlorophenylborane in DME, 2,4,6-triphenyl-boroxin

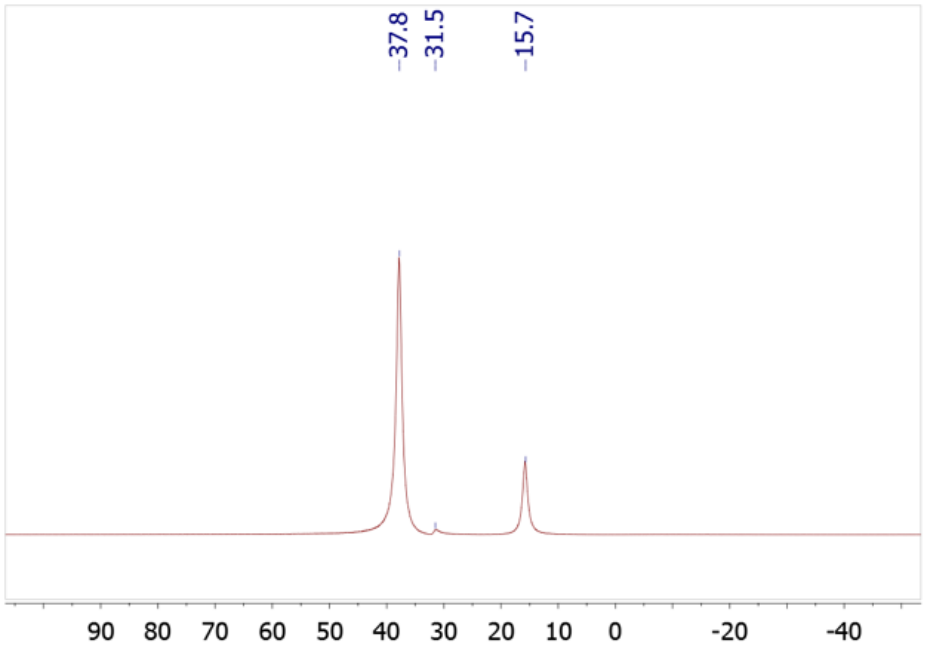
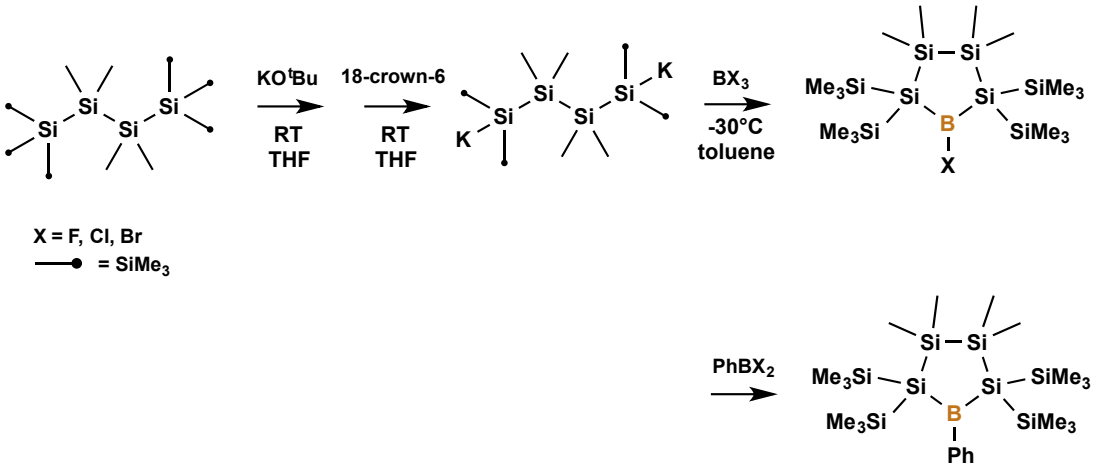


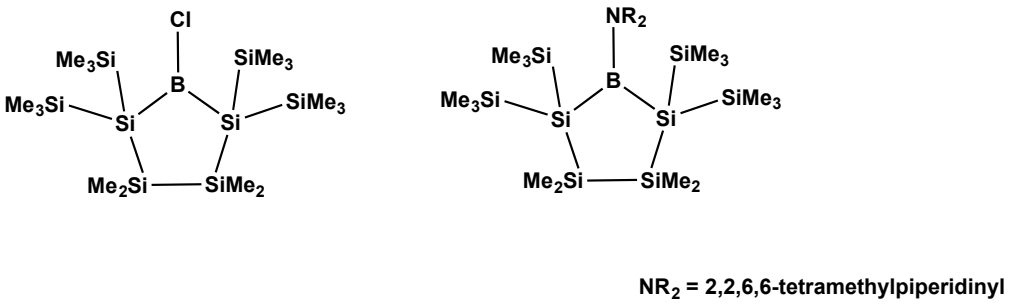
Figure 2.14.: ^{11}B NMR of reaction solution of hypersilylpotassium and dichlorophenylborane in DME, resulting 2,4,6-triphenyl-boroxin

A reaction of the anionic species of 2,2,5,5-tetrakis(trimethylsilyl)decamethylhexasilane, seen in scm.2.6, was reacted with boron halides. Reactions with the BBr_3 only led to product mixtures, and unreacted educt. The reaction with BCl_3 gave colourless oils, with ^{11}B shifts at +80 ppm and ^{29}Si shifts at -5.9, -37.0 ppm and -130.1 ppm. This values can be compared to the literature known compound shown in fig.2.15. Our compound is, compared to the literature data, a little downfield shifted, which could be caused by the chlorine. This would fit to the calculations, which suggested an even more shifted ^{11}B peak of 144.5 ppm (see Table 2.7). To improve crystallisation, reactions with the more cumbrous group, $PhBCl_2$, were carried out (see pathway scm.2.6). The reaction led to an oily slighly yellow residue, which was stored at -30° C for crystallisation. The compound was characterised via ^{11}B and ^{29}Si NMR. A boron shift of +63.1 ppm and the silicon shifts at -10.1 ppm, -12.8 ppm, -82.8 ppm and -122.8 ppm can be compared to literature known data (fig.2.15). Even though the phenyl group on the boron should facilitate the isolation of solid state structures, no crystals could be obtained from the oily product. The instability of the product and the high molecular mass limits the possibilities of analytic methods. However a high-resolution mass spectrometric analysis might gain more product



Scheme 2.6: Pathway 3 reaction to cyclic silylboranes

information.



^{11}B: + 80 ppm
^{29}Si: -5.9 ppm
-37.0 ppm
-130.1 ppm

^{11}B: + 72.1 ppm
^{29}Si: -8.1 ppm
-36.0 ppm
-102.8 ppm

Figure 2.15.: ^{11}B NMR of synthesised chlorosilylborolane and a literature known cyclic silylborane[52]

During the experimental investigation on silylboranes, novel synthetic pathways were sucessfully explored. Especially the reaction of the silyl anion, Hyp-K, with phenyldichlorborane is very auspicious, however reaction conditions still need to be optimised in order to enhance product quality and yield. Isolating greater amounts of the compound Hyp_2PPh is necessary for testing the catalytic ability of the silylborane. By means of NMR, the syntheses of

Table 2.8.: mPW1PW91/Iglo-II (NMR) and mPW1PW91/6-31+G* (optimisation) DFT calculated and experimental data for silylboranes

compound	δ $^{11}B_{calc.}$	$^{1}J_{B\text{-}Ccalc.}$	δ $^{11}B_{exp.}$
BCl_3	49.4		46.50
$PhBCl_2$	53.3	92.8	55.91
Ph_2BCl	62.3	78.1	62.7[96]
Ph3B	64.6	65.6	67.4[97]
HypPhBCl	89.2	70.8	
Hyp_2BPh	142.5	52.0	
		$^{1}J_{B\text{-}Si}$	
$HypBCl_2$	83.2	81.0	
Hyp_2BCl	132.1	59.2	
		59.3	
Hyp_3B	182.8	42.8	
		39.9	
		44.1	
HypPhBCl	89.2	75.0	
Hyp_2BPh	142.5	54.8	
		53.4	
Hyp_2BOTMS	85.6		
CySiBCl	144.5		
$CySiBNMe_2$	66.1		

PhBClHyp can be carried out in the best possible way.
Direct synthesis of the anion with boron halides is more challenging. Due to high reactivity, side products are formed regularly, thats why reaction condition have to be controlled precisely.
The experimental data of the attempts of synthesising cyclic compounds are in line with literature data. Nonetheless the proposed reactions pathway needs to be examined further and more powerful analytic methods are needed for a more precise characterisation of the products.

Looking at the experimental and calculated ^{11}B NMR data, a good agreement in between calculated and experimental data can be detected, which makes the calculation of NMR shifts via DFT a very helpful tool.

2.4. Application of phosphanes and phosphanides for the stabilisation of low valent group 14 compounds

Our calculations showed, that especially phosphanes and phosphanides with silyl substituents, such as TMS and Hyp, are promising for further synthesis of low valent species.

The reaction of PhTMSPH, **3a**, with $SnCl_2$ led to a dark red reaction solution, with a redbrown precipitate. In order to dissolve it and reach complete conversion the solution was refluxed for 2 h. After cooling down slowly, small red crystals could be isolated. These were deluted and showed an ^{31}P NMR shift -132.9 ppm and an ^{119}Sn shift of 1292.6 ppm, with no typical coupling constants. The shifts rather match known Sn-P clusters or Sn-P cubanes, than a diphosphastannylene. A determination of a solid state structure was not possible due to poor crystal quality. The crystals were recrystallized over heptane and stored at -30° C in the dry box.

The reaction of the Hyp substituted compound, PhHypPH **3b**, with $GeCl_2$*dioxane resulted in ^{31}P NMR shifts at -112.4 and -21.4 ppm, calculated values for the germylene, $(PhHypP)_2Ge$, with a planar and a pyramidal P centre, are at 98 and -16 ppm. According to our calculations, substituent combination with Phenyl on P is not suitable to stabilise a monomeric tetrylenes, cone angles of 180° for germylene, 178° are obviously too small.

Reaction of the supermesitylphosphane, (Mes*TMS)PH **4a**, with $GeCl_2$*dioxane shows a ^{31}P NMR shift at 73.2 ppm, which corresponds to the calculated data for this compound, where values at 66 and 32 ppm should be expected for the germylene, (Mes*TMS)P_2Ge **8**. A clear red solution was isolated, which gave a UV-Vis values of 445.

The attempted tetrylene synthesis *via* reaction of the supermesityllithium phospanide, Mes*TMSP-Li **4e**, with the corresponding Sn(II) halides ($SnCl_2$, $SnBr_2$) yielded a dark red solution, and a red-brown precipitate. Further interpretation of this precipitate was difficult due to the poor solubility in any common solvent. While storing the clean red solution in order to gain crystals for a structure determination, yellow crystals could be isolated from this solution. Those were analysed to be Mes*-P=P-Mes* (see Figure 2.10) a side product, which is quite common in the reaction of lithium silylphosphides with halides.[98,99]
As mentioned in literature, reaction with sterically less shielded silylphosphides, such as, Mes*P($SiMe_3$), increases the possibilities of forming a phosphene.[98,99] The P=P distance of 2.054 $\AA$ fits well to previously reported diphosphene structures. The formation of this stable side product seems to be energetically favoured, prohibiting a subsequent reaction with group 14 halogenides to the respective tetrylenes. The red reaction solution, obtained from the reaction of **4e** with the tin halides, was further analyzed *via* NMR where a ^{31}P signal at -392.1 ppm and a ^{119}Sn signal at 1292.3 ppm were detected. Unfortunately, determination of the structure *via* X-Ray diffraction was not possible due to poor quality of the crystals. In literature, a similar NMR pattern for a compound isolated by Westerhausen[100] was found. This compound is a tin-phosphorus cubane with Si^tBu_3 groups on P. This compound shows a ^{31}P signal at -452.1 ppm and a ^{119}Sn peak at 1234.3 ppm with a $^1J_{Sn\text{-}P}$ coupling

constant of 788 Hz and a $^{3}J_{Sn\text{-}P}$ coupling constant of 84 Hz. Thus, it seems that the intramolecular stabilisation *via* the planar P forming a Sn=P double bond is not sufficient to stabilize this stannylene. Further interpretation of the redbrown precipitate was difficult due to the poor solubility in any common solvent. A formation of a decomposition product of the kinetically less shielded stannylene to tin-phosphorus clusters is highly possible. However, a direct reaction of the phosphene with tin bromide led to an immediate color change from yellow to orange-red. This solution was analysed *via* NMR, giving a ^{31}P shift at -347.6 ppm and a small ^{119}Sn shift around 1291 ppm, which again would fit to the formation of a tin-phosphorus cluster or cage-like structure directly from the diphosphene. Since the compound isolated by Westerhausen[100] shows a peak lower than our analysed reaction solution and carbon substituents on P were found to rather form cages, we suppose the formation of multinuclear Sn-P cage structures as mentioned by Wright.[101]

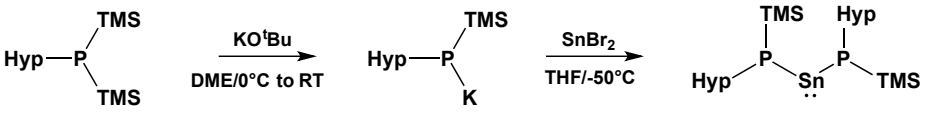
After isolating the clean silylphosphane, [Mes*Si(MeTMS$_2$)P-H] **4b**, further reactions with tin(II) chloride and germanium(II)chloride · dioxane were performed.

Reaction of [Mes*Si(MeTMS$_2$)P-H], **4b**, with ^{n}BuLi and GeCl2 · dioxane led to a red to purple solution. The solution was concentrated and cooled down for crystallisation, no crystals could be obtained. The solution was characterized *via* NMR, ^{31}P shifts of 62.7 ppm and 14.4 ppm were obtained, which compare nicely to calculated values, which are 66.0 ppm and 31.6 ppm. Thus we suppose the formation of the respective germylene. This fits well to the calculated data for the comparable compound **8**, (see Table 2.4).

The compound is a clear red solution, 456 nm, these fit to calculated values for correlating germylenes (416 nm for **8**). Unfortunately, no crystals formed yet.

Hypersilylphosphanes were already preliminary investigated by Hassler[27,102] and Müller,[103,104] where the clean isolation of the isolation of the novel hypersilylphosphanes was approached.

Crystals suitable for X-ray diffraction analysis were obtained after removal of the solvent and recrystallization from toluene with slow evaporation of the solvent at room temperature. The potassium phosphanide crystallises, similar to our Mes* homologues, in a dimeric structural pattern, with a four membered P-K-P-K central ring (see Figure 2.16). Each of the potassium ions is further stabilised *via* a dimethoxyethane molecule and agostic interactions to



TMS = $SiMe_3$
Hyp = $Si(SiMe_3)_3$

Scheme 2.7: Reaction to $Sn(PTMSHyp)_2$

the methyl groups on the hypersilyl moiety. However [HypPK-$SiMe_3$] displays whole molecule disorder.

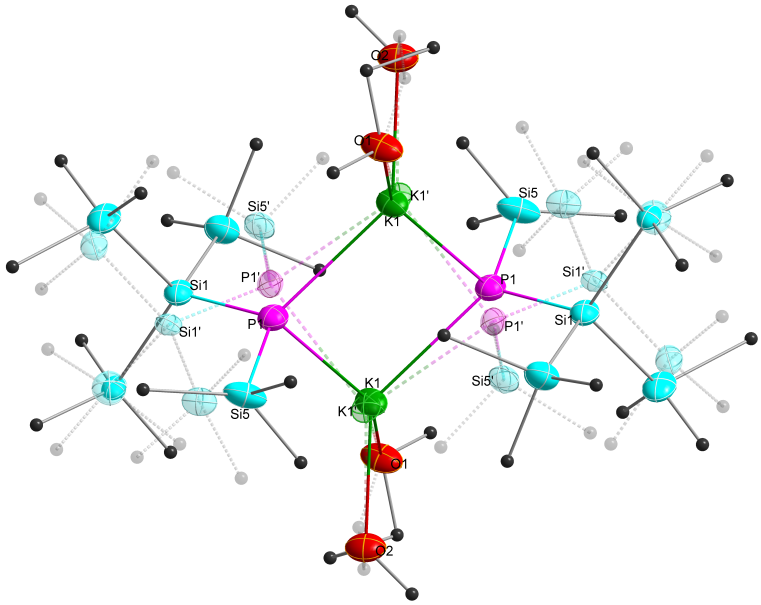


Figure 2.16.: Disordered diagram of dipotassium salt obtained by X-ray diffraction analysis. Hydrogen atoms have been omitted for clarity

Müller used **5a** for the synthesis and isolation of a novel monomeric diphosphastannylene, $(HypTMSP)_2Sn$.[103,105]

The reaction of [HypPK-$SiMe_3$], **5a**, in DME with $GeCl_2$*dioxane deluted in THF to form a germylene led to an immediate change of color to a dark purple. After replacement of the solvents with toluene and filtration, dark red blocks were obtained at low temperatures (-30 °C). UV-Vis measurement of the crystals deluted in toluene was determined with 564 nm and analysis via X-Ray diffraction gave the molecular structure of a novel germaniumcubane, $[(Me_3Si)_3SiPGe]_4$ (see scheme 2.8). The compound crystallises in a trigonal matter in the crystal

system R-3. The average Ge-P-Ge angle is 96.81° and the P-Ge-P angle is in average 82.93°, which means that the cage is a distorted (see Table 2.9). The Hyp substituents are bulky and sterically demanding and can therefore have an influence on the kind/behavior of the P-Ge bonds and angles. The medium P-Ge bond length is about 2.46 $\mathring{A}$, which matches to literature known data for P-Ge single bonds. The ^{31}P shift of -258.6 is more downfield shifted than the values reported for comparable tin-phosphorus cubanes (- 469.8 ppm),[106] however this is the first germanium derivative of this type, and heaving an P-Ge rather than an P-Sn could change the shielding. The ^{29}Si NMR peak at -95.94 (Si($SiMe_3$) ppm with an $^1J_{S\text{-}P}$ coupling constant of 83.5 Hz and a peak at -7.40 ($SiMe_3$) fits to the hypersilyl moiety.

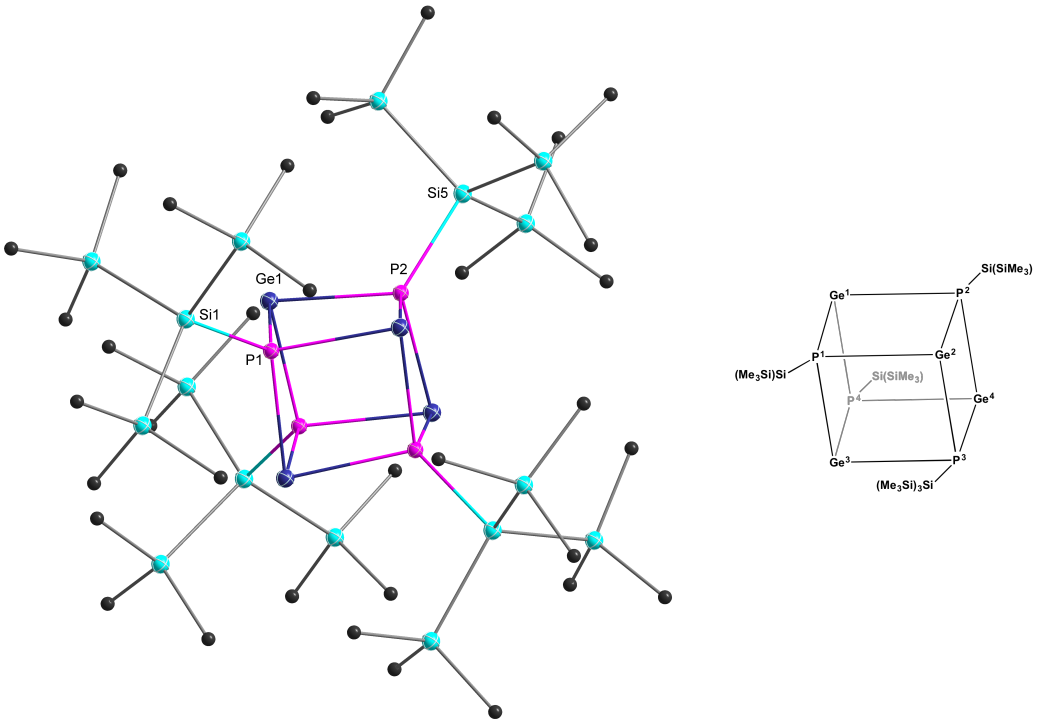
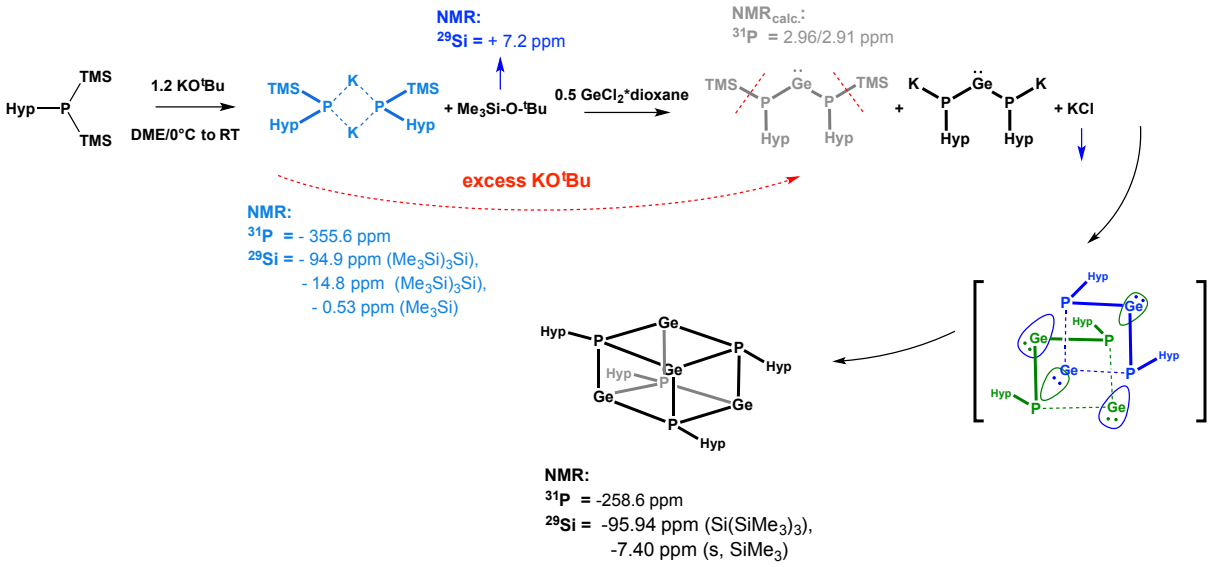


Figure 2.17.: Crystal structure of the novel germaniumcubane **11**

There is just a small number of related compounds known in literature. A tin heterocubane of the similar structure $[(Me_3Si)_3SiPSn]_4$ was isolated by Traut[106] in 2011. This compound was obtained by a reaction of primary silyl phoshines with $SnN(SiMe_3)_2$, a Brønstedt acid base reaction. In contrast, we suspect our germaniumcubane to be formed from the germylene intermediate. Arsenic heterocubanes isolated by Traut[106] show a comparable reaction pathway. Since this germylene was predicted to have enough steric bulk, process



Scheme 2.8: Reaction mechanism germaniumcubane **11**

optimisation might still yield the stable germylene $((HypTMS)P)_2Ge$.

Preliminary reactions to form $((Hyp^tBu)P)_2Sn$, **14**, show tetrylene formation (^{119}Sn = 1592.4 ppm). After two weeks rearrangement to P-Sn clusters seems to occur (^{119}Sn = 1286.3 ppm).

Table 2.9.: mPW1PW91/SDD DFT calculated and experimental data for Ge cubane **11**

Bond lengths	calc. [$\AA$]	exp. [$\AA$]
P1-Si1	2.48	2.44
P2-Si2	2.48	2.44
P3-Si3	2.48	2.47
P4-Si4	2.48	2.44
P1-Ge1	2.48	2.47
P1-Ge2	2.48	2.48
P1-Ge3	2.48	2.47
P2-Ge1	2.48	2.48
P2-Ge2	2.48	2.47
P2-Ge4	2.48	2.48
P3-Ge2	2.48	2.47
P3-Ge3	2.48	2.48
P3-Ge4	2.48	2.47
P4-Ge1	2.48	2.48
P4-Ge3	2.49	2.47
P4-Ge4	2.49	2.48
Bond angles [°]	calc. [°]	exp. [°]
P1-Ge1-P2	96.8	95.4
P1-G2-P2	96.8	95.3
Ge2-P1-Ge1	82.7	84.5
Ge1-P2-Ge2	82.7	84.2
P1-Ge1-P4	96.8	95.8
P1-G3-P4	96.8	96.1
Ge3-P4-Ge1	82.8	83.8
Ge1-P1-Ge3	82.8	88.0
P2-Ge4-P4	96.8	95.4
P4-Ge1-P2	96.8	96.1
Ge1-P2-Ge4	82.7	83.8
Ge1-P4-Ge4	82.8	84.2
P3-Ge4-P2	96.8	95.8
P2-Ge2-P3	96.8	95.3
Ge2-P2-Ge4	82.7	83.8
Ge2-P3-Ge4	82.7	83.8
P2-Ge1-P4	96.8	95.8
P4-Ge4-P2	96.8	96.1
Ge1-P4-Ge4	82.7	83.8
Ge4-P2-Ge1	82.7	83.8
P3-Ge3-P4	96.8	95.3
P4-Ge4-P4	96.8	96.1
Ge3-P4-Ge4	82.7	84.5
Ge4-P3-Ge3	82.7	83.7
^{31}P NMR [ppm]	$\delta_{\text{calc.}}$ [ppm]	$\delta_{\text{exp.}}$ [ppm]
	δ -260, -281	δ -258.6
UV/VIS [nm]	$\delta_{\text{calc.}}$ [ppm]	$\delta_{\text{exp.}}$ [ppm]
	479	564

Chapter 3

Conclusion and Outlook

3.0.1. Conclusion

Through DFT calculations, a series of phosphanes with different characteristics, such as size, steric demand and type of substituent (aryl, alkyl, silyl) were evaluated. The pyramidalisation of the phosphorus atom was evaluated, as this term is suspected to be the main reason for the small number of low valent main group compounds containing phosphorus ligands. A flatter configuration of the P atoms should increase the effective orbital overlap and aid stabilisation.

With calculating the bond angle sums of ΣP of various phosphanes, we could detect a trend in the pyramidalisation of the phosphorus atom. A substitution with ^{t}Bu, TMS and Hyp has a favourable effect on the pyramidalisation of the phosphorus atom than substitution with the comparatively small H or methyl group. Combinations of Mes*PR_2, substituted with silyl ligands (TMS, Hyp) give the highest bond angle sums of ΣP = 351.9°.

Tetrylene configurations with a planar P centre, have a π-type orbital overlap and therefore a stronger stabilisation. NBO analyses, show high delocalisation energies E_2 in the range of 115 - 185 kcal/mol. This interaction causes a shortening of the P-E bond at the planar centre, simultaneously the second P-E bond is significantly elongated.

The compounds $(Mes^*TMS)_2Ge$ and $(Mes^*TMS)_2Sn$ even show minimum structures with two almost planar P centres (346.5/359.9 and 347.0/360.0).

They, however, are the least stable ones. In case of two pyramidal P centres simultaneous interaction between the lone pair of both P centres with the tetrel p-orbital is found, but yields comparably low delocalisation energies (E_2 = 15 - 30 kcal/mol).

For stable tetrylenes additionally, the steric bulk of the ligands has to be considered.
The smaller Phenyl as a backbone, is less likely to shield the active centre, as quite low cone angle values (150° - 170°) were determined.
For $(Mes^*PTMS)_2Sn$ conformers with planar P centres and a cone angle of 176° are found, which according to literature should lead to the isolation of stable stannylene species. In contrast, the combination with Hyp showed better steric shielding (= higher cone angle values 197°) for the active center E.
The Hyp backbone seems the most suitable looking at the steric shielding. In combination with the TMS and ^{t}Bu ligands, cone angles of 197° and 198°, can be achieved. Respectively, making them promising candidates for synthetic evaluation.
In the experimental approach the novel silylphosphanes Ph_2PHyp **3d**, $[Mes^*Si(MeTMS_2)P\text{-}H]$ **4b** and (Mes*Hyp)P-H **4c** were isolated and characterised *via* NMR and single crystal X-ray diffractometry. Additionally two novel silylphosphanides, 2,4,6-tris(*t*-butyl)phenyl trimethylsilyl lithium phosphanide **4e**, [2,4,6-tris(*t*-butyl)phenyl trimethylsilyl potassium phosphanide]·DME **4f** could be isolated and fully characterised.

The isolated silylphosphanes and -phosphanides were used in the attempted synthesis of diphosphatetylenes.

For $[Mes^*Si(MeTMS_2)P]_2Ge$ the NMR and UV/Vis indicate the formation of the desired tetrylene. The synthesis of (HypTMS)P-K with $GeCl_2$*dioxane gave a the first P-Ge cubane of this type instead.
For the stannylenes ^{119}Sn shifts for $[(Mes^*TMS)P]_2Sn$ rather fit to Sn-P clusters. The synthesis of $[Mes^*Si(MeTMS_2)P]_2Sn$, however gave a ^{119}Sn shift of 1549.1 ppm, fitting to a monomeric diphosphastannylene. Crystals for deter-

mining a solid state structure could not be isolated to date.

Silyl anions, which were successful used in the successful isolation of silylphosphanes, were used in the investigation of novel reactions pathways for silylboranes. Those just lately got more attention due to their possible ability of activating hydrogen. Our reaction pathway allows a new approach towards silylboranes. GC-MS showed the formation of the desired product $PhBHyp_2$. However, the recency of those reactions still requires an optimisation of reaction conditions and analytic methods to enable product isolation.

Our combination of calculations and synthetic results indicate that the intramolecular stabilisation *via* formation of E=P (E = Ge, Sn) double bond is less important than previously considered. NBO analysis showed that in conformers with one planar P centre strong π -type interactions occur. At the same time, the second P center is considerably weakened expressed by an elongation of the P-E bond. Consequently steric shielding needs to be increased to ensure stabilisation. For the tetrylenes the HOMO-LUMO gap were determined, giving an idea on their reactivity, since tetrylenes should be highly interesting compounds for complementing transition metal complexes for catalytic purposes. Our tetrylenes have a HOMO-LUMO gap of 2.5 to 3.5 eV, which makes them highly interesting for catalytic investigations and the activation of small molecules, which should be considered for following reactivity studies.

Chapter 4

Experimental Section

4.1. General Procedures

All reactions, unless otherwise stated, were carried out using standard Schlenk line techniques or in a dry box under nitrogen atmosphere. All solvents were dried and deoxygenated by a solvent drying system (Innovative Technology, Inc.). The compounds were stored under inert conditions at room temperature or reduced temperature.

4.1.1. Index of Chemicals

Table 4.1.: Chemicals

1.5

Chemical	CAS	M[g/mol]	ρ [g/mL]	Supplier
n-Butyllithium ^{n}BuLi	109-72-8	64.06	-	Sigma Aldrich 186171
1,2-Dichlorbenzene	195-50-1	147.00	1.3	Merck 102930
Germanium(II)-chloride·dioxane 1:1	28595-67-7	231.65	-	Sigma Aldrich 573515
Lithium aluminium hydride $LiAlH_4$	16853-85-3	37.95	0.92	In-house
Lithium bis(trimethylsilyl)amide	4039-32-1	167.33	0.891	Sigma Aldrich 225770
1,2-Diphosphinobenzene DPB	80510-04-9	142.08	-	ABCR AB130274
Trimethyl phosphate	512-56-1	140.08	-	Sigma Aldrich 241024
Trimethyl phosphite $P(OMe)_3$	121-45-9	124.08	1.052	Sigma Aldrich 240907
Trimethylsilyl chloride	75-77-4	108.64	0.854	Sigma Aldrich 386529
Tin(II)-chloride	7772-99-8	189.61	3.95	Fischer Chemical
Tin(II)-bromide	10031-24-0	278.52	5.12	Sigma Aldrich 309257

4.1.2. NMR

^{1}H (300.2 MHz), ^{13}C (75.5 MHz), ^{29}Si (59.6 MHz) and ^{31}P (121.5 MHz) NMR spectra were recorded on a Mercury 300 MHz spectrometer from Varian at 25°C. Chemical shifts are given in parts per million (ppm) relative to TMS (δ = 0 ppm) regarding ^{1}H, ^{13}C and ^{29}Si, ^{119}Sn relative to $SnMe_4$, for ^{31}P relative to 85% H_3PO_4 and relative to $BF_3{\cdot}OEt_2$ for ^{11}B. Coupling constants *(J)* are reported in Hertz (Hz). All NMR spectra were measured using a D_2O capillary as external lock signal.

4.1.3. X-ray Diffraction

All crystals suitable for single crystal X-ray diffractometry were removed from a Schlenk under inert conditions and immediately covered with a layer of silicone oil. A single crystal was selected, mounted on a glass rod on a copper pin, and placed in the cold N_2 stream provided by Bruker APEX2. For the structure solving the SHELXS97 (Sheldrick 2008) was used, to refine the structure SHELXL2014 (Sheldrick 2014) was used.

4.1.4. Computational details

All calculations have been carried out using the GAUSSIAN09 program package[107] on a computing cluster with blade architecture. For all calculations except calculations of NMR shieldings the mPW1PW91[63] hybrid functional was used. NMR shieldings were calculated using the M06L[108] pure functional as implemented in GAUSSIAN09. For optimisation and calculations of frequencies the 6-31+G* (phosphanes, silylenes) and SDD (germylenes, stannylenes) basis set was used. For calculation of NMR magnetic shieldings the all electron IGLO-II[109] basis set was used (σ ^{1}H = 32.8, σ ^{13}C = 186.2, σ ^{29}Si = 349.5 (TMS),σ ^{11}B = 103.4 ($BF_3.OEt_2$), σ ^{31}P = 624.7 (PH_3), and σ ^{119}Sn = 2721.3 ($Sn(Me)_4$)). The geometries of the molecules were were calculated in the gas phase, without the influence of a solvent. The optimised geometries of all discussed molecules are collected in Appendix A.

4.2. Synthesis

4.2.1. Educts

4.2.1.1. Synthesis of Tetrakis(trimethylsilyl)silane 1

After modified literature:[110] In a flask, attached with a dropping funnel, reflux condenser and bubbler, 100 ml of dry THF are placed and 5 g of lithium were added. Under ice-cooling, trimethylchlorosilane (42.9 mL, 0.34 mol) is added via syringe. Tetrachlorosilane (9.7 mL, 85 mmol, 1: 5 diluted in THF) is slowly added dropwise via the dropping funnel and stirred for a further 12 hours at room temperature. The reaction solution is slowly poured onto 100 ml of 2 M H_2SO_4 / ice and extracted three times with Et_2O. The combined organic phases are dried over Na_2SO_4, filtered through Celite and the solvent removed on a rotary evaporator. After recrystallisation from acetone and filtration 14.9 g (55%) of product are obtained. The product can be sublimed for cleanup.

4.2.1.2. Synthesis of 2,2,5,5-Tetrakis(trimethylsilyl)decamethylhexasilane 2

After modified literature:[111] First step: Synthesis of the silylanion $(SiMe_3)_3Si$-K (Hyp-K)
In order to remove solvent residues and moisture, tetrakis(trimethylsilyl)silan is brought into a Schlenk flask which is then gently heated and flushed with nitrogen for three times. This reaction vessel is brought into the dry box, where 1.1 eq. KOtBu is added. 20 mL DME are added *via* syringe at RT. The colourless solution turns yellow and is stirred overnight at RT. NMR is used to control the progress of the reaction after 2 h.
^{29}Si NMR (DME, D_2O lock, 293 K) δ: -3.93 ppm, -195.83 ppm, (THF, D_2O lock, 293 K) δ: - 4.55, -194.10. Second step:
The solvent is removed under reduced pressure, with that step the product is cleaned from side products (^{t}BuOSiMe$_3$). The residue is redissolving in DME. This solution is transferred with a cannula to a second, cooled (-50° C) vessel with 20 mL of toluene and 0.5 eq tetramethyldichlorosilane. The reaction solution is allowed to warm up to room temperature. This highly voluminous

product is stirred for two hours. For cleanup the solution is poured on 10% HCl/Icewater, the organic layer is isolated and extracted three times with Et2O. The combined organic layers are dried over Na_2SO_4 and the solvent removed on a rotary evaporator. Recrystallisation with ethanol gives a white powder with a melting point of 225-226° C.

4.2.2. Silylphosphanes

4.2.2.1. Synthesis of (PhTMS)P-H 3a

$PhPH_2$ (0.500 g, 4.54 mmol) was dissolved in 20 ml dry Et_2O and cooled to -78° C. ^{n}BuLi (3.40 ml, 5.44 mmol, 1.6 M) is added dropwise via syringe under stirring. The colour changes to yellow. After 30 minutes of stirring at constant temperature, TMS-Cl (0.69 ml, 5.44 mmol) was added slowly via syringe. The colourless solution is stirred over night at room temperature. The solution is filtered and the solvent was removed under reduced pressure. The slightly yellow oil was stored at -30° C for further characterization and further use in following reactions.
NMR data: ^{31}P NMR (C_6D_6, 293 K) δ: -133.2 ($^1J_{P\text{-}H}$ = 210 Hz)

4.2.2.2. Synthesis of (PhHyp)P-H 3b

$PhPH_2$ (0.500 g, 4.54 mmol) was dissolved in 20 ml dry Et_2O and cooled to -78° C. ^{n}BuLi (3.40 ml, 5.44 mmol, 1.6 M) is added dropwise via syringe under stirring. The colour changes to yellow. After 30 minutes of stirring at constant temperature, Hyp-Cl (1.80 ml, 5.43 mmol) was added slowly via syringe. The colourless solution is stirred over night at room temperature. The solution is filtered and the solvent was removed under reduced pressure. The colourless oil was stored at -30° C for further characterization and further use in following reactions.
NMR data for the monomer: ^{1}H NMR (C_6D_6, 293 K) δ: ^{13}C NMR (C_6D_6, 293 K) δ: ^{29}Si NMR (C_6D_6, 293 K) δ: -9.92 ppm ppm (-Si(**Si**$Me_3)_3$), $^2J_{Si\text{-}P}$ = 13 Hz), -80.21 ppm ((-**Si**$(SiMe_3)_3$), $^1J_{Si\text{-}P}$ = 104.0 Hz) ^{31}P NMR (C_6D_6, 293 K) δ: -137.3 ($^1J_{P\text{-}H}$ = 200 Hz)

4.2.2.3. Synthesis of $PhPHyp_2$ 3c

KO^tBu (1.30 g, 9.97 mmol) and tetrakis(trimethylsilyl)silane (3.20 g, 11.6 mmol) were stirred in 40 mL of dry DME at 0° C for 2h. Dichlorophenylphosphane (0.68 mL, 5.00 mmol) was dissolved in 20 mL of dry DME and the dark yellow Hyp–K solution from step 1 was added dropwise via syringe at -30° C. The mixture was allowed to warm up to rt was stirred over night. A colourless precipitate formed, it was removed via filtration. The solvents were evaporated and the residue was attempted to recrystallize from toluene and heptane. Interestingly using metal capillary for filtration leads to a decomposition of the phosphane, and only the disilane was detectable by NMR. Filtration with Celite gives a clear product, which is a mixture of the dimeric and the monomeric compound.
NMR data for the monomer: ^{29}Si NMR (C_6D_6, 293 K) δ: -10.35 ppm ppm (-Si(**Si**$Me_3)_3$), $^2J_{Si\text{-}P}$ = 9 Hz), -94.82 ppm ((-**Si**$(SiMe_3)_3$), $^1J_{Si\text{-}P}$ = 86.0 Hz) ^{31}P NMR (C_6D_6, 293 K) δ: -132.9 ppm

4.2.2.4. Synthesis of Ph_2PHyp 3d

20 ml of dry Et_2O were added to Ph_2PH (0.50 ml, 2.87 mmol) and cooled to -78° C. ^{n}BuLi is added dropwise via syringe and the yellow solution was stirred for 30 minutes at constant temperature. Hyp-Cl (1.15 ml, 3.47 mmol) was added slowly via syringe. The pale-yellow solution is allowed to warm up to room temperature and was stirred overnight. The solution is filtered the next day, and the solvent is removed under reduced pressure. 5 ml of dry heptane were added for clean up, followed by another filtration. The product is stored at 0° C, crystals suitable for X-ray difraction analysis were isolated.
textsuperscript1H NMR (C_6D_6, 293 K) δ: ^{13}C NMR (C_6D_6, 293 K) δ: ^{29}Si NMR (C_6D_6, 293 K) δ: -9.74 ppm ppm (-Si(**Si**$Me_3)_3$), $^2J_{Si\text{-}P}$ = 12.0 Hz), -88.91 ppm ((-**Si**$(SiMe_3)_3$), $^1J_{Si\text{-}P}$ = 73.0 Hz,) ^{31}P NMR (C_6D_6, 293 K) δ: -57.0

4.2.2.5. Synthesis of (Mes*TMS)P-H 4a

Mes*PH2 (0.50g, 1.80mmol) was dissolved in 20mL dry Et_2O and cooled to -78° C. ^{n}BuLi (0.86 mL, 2.16 mmol), 2.5 m) was added dropwise to the solution

via syringe, to the slightly yellow solution, trimethylchlorosilane (0.27 mL, 1.80 mmol) was added dropwise via syringe at -78° C. The solution was allowed to warm up to room temperature and was stirred over night, a colourless, solid precipitate formed (LiCl). After filtering off the salts and removing the solvent the pale yellow, oily residue was redissolved in 20mL of dry toluene and stored at -30° C, no crystals suitable for further characterisation were isolated.
^{1}H NMR (C_6D_6, 293 K) δ: 7.01 (Mes*), 1.37 (^{t}Bu), 0.12 (Si(SiC**H**$_3$)$_3$) ^{13}C NMR (C_6D_6, 293 K) δ: 123.8 ppm, 148.2 ppm, 155.3 ppm (Mes*-), 33.4, 38.9 (^{t}Bu), 3.4 (Si(Si**C**H$_3$) ^{29}Si NMR (C_6D_6, 293 K) δ: 8.85 ppm (TMS, $^{1}J_{Si\text{-}P}$ = 21.2 Hz) ^{31}P NMR (C_6D_6, 293 K) δ: -128.9 ppm ($^{1}J_{P\text{-}H}$ = 212.0 Hz)

4.2.2.6. Synthesis of [Mes*Si(MeTMS$_2$)P-H] 4b

Mes*PH$_2$ (0.50 g, 1.80 mmol) was dissolved in 20 mL of dry Et$_2$O and cooled to -78° C and ^{n}BuLi (0.86 mL, 2.16 mmol) was added dropwise via syringe, while the solution turns yellow. The reaction was stirred for 30 min at -78° C, 2-chloroheptamethyltrisilane (0.57mL, 2.16mmol) was added slowly via syringe at -78° C, after that the reaction is allowed to warm up to room temperature. It was stirred overnight. The solution turns colourless with formation of an colourless precipitate (LiCl). After filtration, the solvent was removed under reduced pressure. The residue was redissolved in 20mL of dry toluene. Crystals suitable for X-ray characterisation formed after storing the yellow oil at -30°
^{1}H NMR (C_6D_6, 293 K) δ: 7.2 (Mes*), 1.37 (^{t}Bu), 0.19 (Si(SiC**H**$_3$)$_3$) ^{13}C NMR (C_6D_6, 293 K) δ: 121.8 ppm, 147.8 ppm, 154.8 ppm (Mes*-), 33.4, 38.9 (^{t}Bu), -17.0 (Si-**C**H$_3$), 5.3 (Si(Si**C**H$_3$)$_3$) ^{29}Si NMR (C_6D_6, 293 K) δ: 7.40 ppm (TMS3, $^{1}J_{Si\text{-}P}$ = 71.0 Hz), -50.62 (Hyp, $^{1}J_{Si\text{-}P}$ = 71.0 Hz, $^{2}J_{Si\text{-}P}$ = 17.5 Hz) ^{31}P NMR (C_6D_6, 293 K) δ: -127.2 ppm ($^{1}J_{P\text{-}H}$ = 221.8 Hz)

4.2.2.7. Synthesis of (Mes*Hyp)P-H 4c

Mes*PH$_2$ (0.50 g, 1.80 mmol) was dissolved in 20 mL of dry Et$_2$O and cooled to -78° C. ^{n}BuLi (0.86 mL, 2.16 mmol, 2.5 m) was added dropwise via syringe, while the solution turns yellow. The reaction was stirred for 30 min at -78 ° C, Hyp – Cl (0.60 mL, 1.80 mmol) was added dropwise via syringe at -78° C. A colour change form yellow over orange to reddish brown occurs. The reac-

tion solution is allowed to warm up to room temperature and was stirred over night, while it turns colourless and a colourless precipitate (LiCl) formed. The solid was filtered, and solvents were removed under reduced pressure. A light brown oil remained. This residue was redissolved in 20mL of dry toluene. Crystals suitable for X-ray characterisation formed at storing the yellow oil at -30° C.
^{1}H NMR (C_6D_6, 293 K) δ: 7.12 (Mes*), 1.34 (^{t}Bu), 0.12 (Si(SiC**H**$_3$)$_3$) ^{13}C NMR (C_6D_6, 293 K) δ: 122.7 ppm, 147.9 ppm, 155.1 ppm (Mes*-), 32.4, 37.9 (^{t}Bu), -17.0 (Si-**C**H$_3$), 5.3 (Si(Si**C**H$_3$)$_3$) ^{29}Si NMR (C_6D_6, 293 K) δ: 7.50 ppm (-Si(**Si**Me$_3$)$_3$), -83.00, -9.50 ((-**Si**(SiMe$_3$)$_3$) $^{1}J_{Si-P}$ = 67.5 Hz, $^{2}J_{Si-P}$ = 5.62 Hz) ^{31}P NMR (C_6D_6, 293 K) δ: -137.8 ppm ($^{1}J_{P-H}$ = 220.6 Hz)

4.2.2.8. Synthesis of Mes*PTMS$_2$ 4d

Mes*PH2 (0.50g, 1.80mmol) was dissolved in 20mL dry Et_2O and cooled to -78° C. ^{n}BuLi (0.86 mL, 2.16 mmol), 2.5 m) was added dropwise to the solution via syringe, to the slightly yellow solution, trimethylchlorosilane (0.27 mL, 1.80 mmol) was added dropwise via syringe at -78° C. The solution was allowed to warm up to room temperature and was stirred over night, a colourless, solid precipitate formed (LiCl). The solution was cooled down -78° C. The same amounts of ^{n}BuLi (0.86 mL, 2.16 mmol), 2.5 m) and trimethylchlorosilane (0.27 mL, 1.80 mmol) as in the first step were slowly added. The solution turns yellow again. After adding of TMS-Cl the solution is allowed to warm up to room temperature and was stirred over night. Again a colourless, solid precipitate formed (LiCl). After filtering off all of the salts and removing the solvent the colourless, oily residue was redissolved in 10mL of dry toluene and stored at -30° C, no crystals suitable for further characterisation were isolated.
^{29}Si NMR (C_6D_6, 293 K) δ: 5.50 ppm (dubl.tripl.) ^{31}P NMR (C_6D_6, 293 K) δ: 146.0 ppm

After filtering off the salts and removing the solvent the pale yellow, oily residue was redissolved in 20mL of dry toluene and stored at -30° C, no crystals suitable for further characterisation were isolated.

4.2.3. Phosphanides

4.2.3.1. Synthesis of 2,4,6-tris(*t*-butyl)phenyl trimethylsilyl lithium phosphanide 4e

2,4,6-tris(*t*-butyl)phenyl trimethylsilyl phosphane (0.40 g, 1.14 mmol) is dissolved in 5 mL of THF. 0.82 mL of 1.6 M *n*-butyl lithium (1.15 eq, 1.31 mmol) in hexanes is added dropwise at RT. The colour of the reaction solution changes to yellow and the solution is stirred for additional 2h. After evaporation of all volatile components, the solid residue is redissolved in *n*-hexane. After one week at -30 °C, crystals suitable for X-ray diffraction analysis can be isolated from this solution. Isolated yield: 0.19 g, 42%.
^{1}H NMR (C_6D_6, 293 K) δ: 0.15 ppm (9H, d, $SiMe_3$, $^{3}J_{HP}$ = 3.9 Hz), 3.04 ppm (18H, o-*t*-Bu) 3.11 ppm (9H, p-*t*-Bu) 7.19 ppm (2H, d, arom., $^{4}J_{HP}$ = 1.8 Hz). ^{13}C NMR (C_6D_6, 293 K) δ: 4.0 ppm ($SiMe_3$, d, $^{2}J_{CP}$ = 12.8 Hz), 31.2 ppm (o-C*Me$_3$*, d, $^{3}J_{CP}$ = 8.1 Hz), 33.4 ppm (o-*C*Me$_3$, d, $^{4}J_{CP}$ = 8.8 Hz), 34.5 ppm (p-C*Me$_3$*), 38.5 ppm (p-*C*Me$_3$), 118.5 ppm (arom., d, $^{2}J_{CP}$ = 3.7 Hz), 118.9 ppm (arom.), 149.5 ppm (arom.), 157.1 ppm (arom.). ^{29}Si NMR (C_6D_6, 293 K) δ: 7.94 ppm (d, $^{1}J_{SiP}$ = 21.8 Hz). ^{31}P NMR (C_6D_6, 293 K) δ: -151.4 ppm.

4.2.3.2. Synthesis of [2,4,6-tris(*t*-butyl)phenyl trimethylsilyl potassium phosphanide]·DME 4f

0.13 g (0.28 mmol) of 2,4,6-tris(*t*-butyl)phenyl bis-trimethylsilyl phosphane are dissolved in 3 mL of DME. A solution of 0.035 g (0.31 mmol) of KO*t*Bu in 2 mL of DME is added dropwise at RT. The colourless solution changes to yellow immediately and is subsequently stirred for 2h. After evaporation of all volatile components, the residue is redissolved in *n*-hexane. After one week at -30 °C, crystals suitable for X-ray diffraction analysis could be isolated from this solution. Isolated Yield: 0.11 g, 82%
^{1}H NMR (C_6D_6, 293 K) δ: 0.16 ppm (9H, d, $SiMe_3$, $^{3}J_{HP}$ = 3.4 Hz), 1.46 ppm (9H, p-*t*-Bu) 1.99 ppm (18H, o-*t*-Bu) 2.96 ppm (6H, DME CH_3) 3.00 ppm (4H, DME CH_2) 7.50 ppm (2H, broad s, arom.). ^{13}C NMR (C_6D_6, 293 K) δ: 4.0 ppm ($SiMe_3$, d, $^{2}J_{CP}$ = 12.8 Hz), 31.2 ppm (o-C*Me$_3$*, d, $^{3}J_{CP}$ = 8.1 Hz), 33.4 ppm (o-*C*Me$_3$, d, $^{4}J_{CP}$ = 8.8 Hz), 34.5 ppm (p-C*Me$_3$*), 38.5 ppm (p-*C*Me$_3$), 58.3 ppm

(DME) 71.0 ppm (DME) 118.8 ppm (arom., d, $^{2}J_{CP}$ = 12.8 Hz), 118.9 ppm (arom.), 143.4 ppm (arom.), 155.9 ppm (arom.). ^{29}Si NMR (C_6D_6, 293 K) δ: -0.70 ppm (d, $^{1}J_{SiP}$ = 58.4 Hz). ^{31}P NMR (C_6D_6, 293 K) δ: -142.4 ppm.

4.2.3.3. Synthesis of [HypP(SiMe$_3$)K·DME] 5a

1.00 g (2.4 mmol) HypP(SiMe$_3$)$_2$ and 0.28 g (2.5 mmol) of KO^{t}Bu are brought into a Schlenk flask under inert atmosphere. Dissolution of the solid, colourless educts in 6 mL of 1,2-Dimethoxyethane (DME) at 0°C led to an immediate change of colour to intense yellow. After vigorous stirring for 24 h all volatile components were removed under reduced pressure. The residue was redissolved in a mixture of pentane and toluene. Crystals suitable for X-Ray diffraction analysis were obtained from this solution at -30° C. Yield: 0.98 g, 87%.
^{1}H NMR (C_6D_6, 293K): δ 0.09 ppm (27H, s, (*Me$_3$*Si)$_3$Si) 0.17 (9H, broad s, *Me$_3$*Si). ^{13}C NMR (C_6D_6, 293K): δ 2.0 ppm (9C, d, $^{3}J_{CP}$ = 12.2 Hz, (*Me$_3$*Si)$_3$Si), 8.5 ppm (3C, d, $^{2}J_{CP}$ = 11.6 Hz, *Me$_3$*Si). ^{29}Si NMR (C_6D_6, 293K): δ -94.9 ppm (Si, d, $^{1}J_{SiP}$ = 118.2 Hz, (Me$_3$Si)$_3$*Si*), -14.8 ppm (3Si, d, $^{2}J_{SiP}$ = 11.4 Hz (Me$_3$*Si*)$_3$Si), -0.53 ppm (1Si, d, $^{1}J_{SiP}$ = 78.9 Hz, Me$_3$*Si*). ^{31}P NMR (C_6D_6, 293 K): δ -355.6 ppm.

4.2.4. Silylboranes

4.2.4.1. Synthesis of Hyp$_2$BCl 6a

1.00 g (3.12 mmol) of tetrakis(trimethylsilyl)silane are weighed into a Schlenk flask under inert atmosphere. The flask is carefully heated 3 times and brought into the dry box. 0.384 g (3.42 mmol) of KO^{t}Bu are added. Subsequently, 20 mL THF is added *via* syringe, the solution turns abruptly yellow and is stirred at 60 °C for 2 h. The conversion of the reaction and the formation of the silyl anion was controlled after 2 h *via* ^{29}Si NMR.
^{29}Si NMR (C_6D_6, 293K): δ -4.55 ppm, -194.10 (K-*Si*(SiMe$_3$)$_3$
All volatile components were removed under reduced pressure and 20 ml of toluene were added. BCl_3 is added to 20 ml cooled (0 °C) hexane and cooles down to -75°C. HypK form step 1 was addes slowly *via* filter cannula. After complete addition, the ethanol/N_2 cooling bath was removed and the reaction

solution is allowed to warm up to room temperature. (Attention when removing the filter cannula, HypK pyrophoric!) The solution turns colourless and a precipitate forms, which was filtered off with Celite, the solvent was removed under reduced pressure and the resulting slightly yellow oil was stored in the glove box at -30 °C.

This reaction was prepared in three different stoichiometric ratios: 1:1 (HypK:BCl_3):

colourless solution, after the filtration white grease like solid formed at -30 °C.

^{11}B (D_2O): 82 ppm (small), 50 ppm (small), 23 ppm, 18 ppm

^{29}Si (D_2O): -10.3 ppm (1.4), -10.5 ppm (0.25), -13.2 ppm (1), -82.0 ppm, -82.2 ppm

GC-MS:

$Hyp_2BOSiMe_3$ M^+ = 593

Hyp_2BR M^+ = 255 (Cl, B) main product

HypH M^+ = 248

1:2 (HypK:BCl_3):

colourless viscous oil

^{11}B (D_2O): 82 ppm, 35.6 ppm, 20 ppm (small)

^{29}Si (D_2O): -10.3 ppm (0.6), -10.5 ppm (0.4), -13.2 ppm (1), -82.0 ppm, -82.2 ppm

GC-MS:

$Hyp_2BOSiMe_3$ M^+ = 593

Hyp_2BR M^+ = 669 (Cl, B) main product

HypR M^+ = 305

1:3 (HypK:BCl_3):

Pale brown viscous oil

^{11}B (D_2O): 82 ppm, 20 ppm (small)

^{29}Si (D_2O): -10.3 ppm (0.6), -13.2 ppm (1), -82.0 ppm

4.2.4.2. Synthesis of Hyp_2BPh 6b

2.2 g (6.86 mmol) of tetrakis(trimethylsilyl)silane are weighed into a Schlenk flask under inert atmosphere. The flask is carefully heated 3 times and brought into the dry box. 0.768 g (6.84 mmol) of KO^tBu are added. Subsequently, 20 mL THF is added *via* syringe, the solution turns abruptly yellow and is stirred

at 60 °C for 2 h. The conversion of the reaction and the formation of the silyl anion was controlled after 2 h *via* ^{29}Si NMR.
^{29}Si NMR (C_6D_6, 293K): δ -4.55 ppm, -194.10 (K-*Si*($SiMe_3$)$_3$
All volatile components were removed under reduced pressure and 20 ml of toluene were added and this solutions was cooled to -30°C. $PhBCl_3$ (0.44 g, 0.36 mL, 2.8mmol) in hexanes (cooled to 0°C) was deluted in 20 ml toluene and cooled to -30°C. HypK from step 1 was slowly added *via* filter cannula. After complete addition, the ethanol/N_2 cooling bath was removed and the reaction solution is allowed to warm up to room temperature. (Attention when removing the filter cannula, HypK pyrophoric!) The solution turns colourless and a precipitate forms, which was filtered off with Celite, the solvent was removed under reduced pressure and the resulting colourless oil was stored at -80 °C.
2:1 (HypK : $PhBCl_2$):
colourless solution, after the filtration white grease like solid formed at -30 °C.
^{11}B (D_2O): 64 ppm, 30 ppm
^{29}Si (D_2O): -10.5 ppm (0.6), -12.3 ppm (0.15), -13.5 ppm (1), -82.5 ppm
GC-MS:
Hyp_2BPh M^+ = 583 main product
(60 % formation) HypCl M^+ = 282
HypH M^+ = 247

4.2.4.3. Synthesis of cyclic silylboranes 6c and 6d

Reaction of decasilanide with BCl_3

0.50 g (8.2 mmol) of decasilane are weighed into a Schlenk flask and were carefully heated and flushed with nitrogen for 3 times. The flask is brought into the dry box and 0.197 g (1.76 mmol) of KO^{t}Bu and 0.451 g (1.71 mmol) of crown ether were added. Subsequently, 20 mL THF added by syringe at room temperature, the solution turns yellow and was stirred overnight at RT. The conversion of the reaction was audited *via* NMR.
^{29}Si NMR (C_6D_6, 293K): δ -9.95 ppm, -29.0, -126.5
All volatile components were removed under reduced pressure and 20 ml of toluene were added. BCl^3 were added to a cooled solution (0 °C) of 10 mL of toluene and 10% of Et^3N. This solution was added *via* syringe to the anion

prepared in step 1 at -30 °C. After complete addition, the cooling bath was removed and the solution was stirred over night at RT. The resulting salts were seperated over Celite, the clear solution was stored at -30 °C. Crystals formed after two days, which were analysed to be crown ether, after removing those crystals the solution was stored at -30 °C in the dry box.
^{11}B (C_6D_6): 80 ppm (broad), 1.4 ppm
^{29}Si (C_6D_6): 7.4 ppm, -5.9 ppm, -37.0 ppm, -130.1 ppm

Reaction of decasilanide with $PhBCl_2$
1.00 g (1.64 mmol) of decasilane are weighed into a Schlenk flask and were carefully heated and flushed with nitrogen for 3 times. The flask is brought into the dry box and 0.408g (3.64 mmol) of KO^tBu were added. Subsequently, 20 mL THF added by syringe at room temperature, the solution turns yellow and was stirred overnight at RT. NMR for reaction control. ^{29}Si NMR (C_6D_6, 293K): δ -9.95 ppm, -29.0, -126.5
All volatile components were removed under reduced pressure and 20 ml of toluene were added. $PhBCl_2$ (0.20 g, 0.17 ml, 1.25 mmol) were added to 10 mL cooled toluene (0 °C). The anion from step 1 was added *via* filter canulla at -30 °C. After complete addition, the cooling bath was removed and the solution was stirred over night at RT. The resulting salts were separated over Celite, the clear solution was stored at -30 °C.
^{11}B (C_6D_6): 63.1 ppm, 3.8
^{29}Si (C_6D_6): -10.1 ppm, -12.8 ppm, -82.8 ppm, -122.8 ppm

4.2.5. Tetrylenes

4.2.5.1. Germylenes

4.2.5.2. Synthesis of $(PhHypP)_2Ge$ 7

Product **3b** was deluted in 15 ml of dry Et_2O. The solution is cooled to -30°C and $_n$BuLi (3.9 ml, 6.24 mmol) is added drop-wise via syringe. $GeCl_2$·dioxane (0.590 g, 4.11 mmol) was dissolved in 5 ml dry THF in a separate flask. After

stirring both solutions for 30 minutes, **3b** is added to $GeCl_2$·dioxan (in THF) dropwise via syringe, the solution turned dark red and was stirred at rt over night. Afterwards the solution was filtered and stored at -30°C.
^{1}H NMR (C_6D_6, 293K): δ 0.089 ppm (hydrogen atoms of methyl groups), 6.85/7.0 ppm (of benzene), 7.51 ppm (of benzene) ^{29}Si NMR (C_6D_6, 293K): δ -94.82 ppm (d, **Si**($SiMe_3$, $^{1}J_{P\text{-}Si}$ = 86.8 Hz, -10.35 ppm (Si(**Si**Me_3, $^{2}J_{P\text{-}Si}$ = 8.8 Hz)) ^{31}P NMR (C_6D_6, 293 K): δ -112.4 ppm, - 21.2 ppm (small), -142.3 ppm (educt)

4.2.5.3. Synthesis of $(Mes^*TMSP)_2Ge$ 8

0.5 g (1.40 mmol) of the oily product **4a** was dissolved in 15 ml 15 ml of dry Et_2O, the solution is cooled to -30°C and ^{n}BuLi (0.67 ml, 1.68 mmol) is added dropwise via syringe. $GeCl_2$·dioxane (0.15 g, 0.66 mmol) was dissolved in 10 mL of dry THF and added dropwise via cannula at -78°C. The mixture was allowed to slowly warm up to rt, and was stirred for 12 h. The colour changed to a dark red. Solvent was partly removed under reduced pressure and and the the oily residue was redissolved in toluene. The product was stored at -30°C.
^{29}Si NMR (C_6D_6, 293K): δ 5.42 ppm (**Si**Me_3, $^{1}J_{P\text{-}Si}$ = 8.8 Hz)) ^{31}P NMR (C_6D_6, 293 K): δ 73.19 ppm, -129.2 ppm ppm (educt) UV-Vis: 445 nm

4.2.5.4. Synthesis of $[Mes^*Si(Me(SiMe_2)_2))P]_2Ge$ 9

Product **4b** was redissolved in 20 mL of pentane and was cooled to 78°C. ^{n}BuLi (0.56 mL, 1.40 mmol, 2.5 m) was added dropwise via syringe where the colour changed to yellow. After 45 min of stirring GeCl2 · dioxane (0.155 g,0.67 mmol) in THF was added dropwise. The colour turned darker. After stirring over night a sample for NMR spectroscopy was taken. The salts were removed via filtration, the solvents were removed under reduced pressure and the residue was stored for crystallisation at rt and later at -30°C.
^{29}Si NMR (C_6D_6, 293K): δ ^{31}P NMR (C_6D_6, 293 K): δ 62.7 ppm, 14.4 ppm UV-Vis: 456 nm

4.2.5.5. Synthesis of $(Mes^*_2P)_2Ge$ 10

Step 1: Mes*Br (1.16g, 3.57mmol) was dissolved in 25mL of dry Et_2O and cooled to -30°C. ^{n}BuLi(1.58mL, 3.92mmol, 2.5m) was added dropwise via syringe. After stirring for 45 min at 30°C, PCl_3 (0.16 mL, 3.57 mmol = 1.57 g/mL) was added dropwise via syringe. The mixture was allowed to warm up to RT and stirred over night. The solvent was removed under reduced pressure. The yellow, solid residue was redissolved in dry Et_2O and was addes slowly to a cooled (0°C) $LiAlH_4$ (0.07 g, 1.79 mmol) solution in 20 mL of dry Et_2O. The greyish-yellow, cloudy reactions solution was stirred over night at RT. The reaction was transformed via cannula into a 10mL degased H_2O:HCl (90:10) solution. The organic layer was separated from the aqueous phase and dried over Na_2SO_4. After removing the drying agent via filtration, the solvent was removed under reduced pressure. The residue was a pale yellow powder. The product was characterised via GC-MS. Step 2: The resulting yellow solid was redissolved in hexane. The solution was lithiated using 4.31 mL (10.77 mmol, 2.5 m) ^{n}BuLi and stirred for 45 min at -30°C. $GeCl_2$·dioxane (0.35 g 4.49 mmol) (dissolved in dry THF) was added dropwise via cannula at -78°C. While stirring over night at RT the mixture turned yellow and a colourless, solid precipitate formed. The solid removed via filtration and the yellow solution was stored for further characterisation. Small orange crystals were formen, however with poor diffracting quality.
^{29}Si NMR (C_6D_6, 293K): δ -50.62 ppm (**Si**$(Me(SiMe)_2)$, $^1J_{P\text{-}Si}$ = 52.8 Hz)) ^{31}P NMR (C_6D_6, 293 K): δ 24.8 ppm

4.2.5.6. Synthesis of a novel P-Ge cubane 11

A solution of HypP(SiMe3)K.DME (1 g, 2.07 mmol) in 6 mL of DME was cooled to -50 ° C and slowly added to a cooled (-50 ° C) suspension of $GeCl_2$.dioxane (0.24g, 1.0 mmol) in 10 mL of THF in a 100 mL Schlenk flask via cannula under vigorous stirring. Upon addition the reaction solution turned purple. The reaction was allowed to warm up to room temperature and was vigorously stirred for 16 hours. After removal of solvents under reduced pressure the residue was dissolved in pentane and filtered from salts. Dark red crystals suitable for X-Ray diffraction analysis were obtained from pentane at -30 ° C. Yield: 0.21

g, 76%
^{1}H NMR (C_6D_6, 293 K): δ 1.30 ppm (broad s, (Me_3Si)$_3$Si). ^{31}P NMR (C_6D_6, 293 K):δ -258.6 ppm ^{29}Si NMR (C_6D_6, 293 K): δ -95.94 ppm (d, $^{1}J_{SiP}$ = 83.5 Hz, Si(SiMe3)3), δ -7.40 ppm [s, SiMe3]. UV-VIS: 564 nm

4.2.5.7. Stannylenes

4.2.5.8. Synthesis of (PhHypP)$_2$Sn 12

15 ml Et_2O (dry) are added to the flask with product **3b** (1.52 g, 4.3 mmol) the solution is cooled to -78°C. ^{n}BuLi (3.20 ml, 5.12 mmol) is added dropwise via syringe and solution was stirred for 45 minutes at constant temperature. $SnCl_2$ (0.398 g, 2.099 mmol) was dissolved in 5 ml of dry THF and also cooled to -78°C and the etheric solution of (PhHyp)P-H was added via canulla. Bright red colouring can be observed. The solution is stirred for 30 minutes at constant temperature and under shading (aluminum foil) before it is stored at -30℃. Solution is heated (reflux) for 5 h and afterwards stored at rt and -30℃. Dark red crystals can be observed at -30℃.
^{1}H NMR (C_6D_6, 293 K): δ ^{13}C NMR (C_6D_6, 293 K): δ ^{29}Si NMR (C_6D_6, 293 K): δ
^{31}P NMR (C_6D_6, 293 K): δ -132.9 ppm (no P-Sn coupling constants detected)
^{119}Sn NMR (C_6D_6, 293 K): δ 1292.6 ppm

4.2.5.9. Synthesis of [Mes*Si(MeTMS$_2$)P]$_2$Sn 13

2 reaction pathways: Pathway 1: A solution of **4c** (0.11 g, 2.10 mmol) in 20 mL of toluene was cooled to -75°C. Sn[N(TMS)$_2$]$_2$ (0.20 mL, 1.08 mmol) was added drop-wise via syringe at -75°C, dark yellow colour occurs during the reaction. The cooling was removed and the mixture was stirred over night at rt, a colour change to a light orange was detected.
NMR ^{31}P NMR (C_6D_6, 293 K): δ -127.36 ppm ^{119}Sn NMR (C_6D_6, 293 K): δ 1549.1, 1293.4 ppm (small)

Pathway 2: A solution of **4c** (0.2 g, 3.81 mmol) in 20 mL of dry Et_2O was cooled to -78°C and lithiated with ^{n}BuLi (2.85 ml, 4.5 mmol), further a reaction with 2-chloroheptamethyltrisilane led to the formation of Mes*PHyp2. All

salts were removed via filtration, the solvent was removed under reduced pressure and the residue was redissolved in 20 mL of dry pentane. KO^{t}Bu (0.25g, 2.16mmol) (dissolved in dry DME) was added drop-wise via cannula at 0°C, where a colourchange to dark orange occured. The mixture was stirred over night at RT. Solvent was removed under reduced pressure until a purple, oily residue was left. The residue was redissolved in 20 mL of dry pentane and $SnBr_2$ (0.24 g, 0.90 mmol) (dissolved in 20 mL of dry THF) was added drop-wise via cannula. The mixture turned dark red, a darkbrown precipitate was formed and the solution turned cloudy. The precipitate was filtered off and was stored for further analysis.
^{31}P NMR (C_6D_6, 293 K): δ -127.30 ppm (no P-Sn coupling constants detected)
^{119}Sn NMR (C_6D_6, 293 K): δ 1293.4 ppm

4.2.5.10. Synthesis of [^{t}BuHypP]$_2$Sn 14

Preparation of ^{t}BuHyp$_2$P A one step reaction to form the product ^{t}Bu$_2$PHyp, from ^{t}PCl$_2$ and 2 eq KO^{t}Bu, equivalent to Ph$_2$PHyp, leads to a mixture of the monomeric and the dimeric phosphane ^{t}BuHypP-PHyp^{t}Bu in a ratio of approximately 1:3. Also on the two step reaction there is always a mixture of both compounds detected, however the 2 step pathway leads to the monomer as main product, the determination of a crystal structure was not possible due to high reactivity of the monomer.
Two step pathway:
^{t}BuPCl$_2$ (5.00 mL, 5.00 mmol, 1 m) was dissolved in 10 mL of dry DME and was added to a previous prepared solution of the anion, Hyp-K (1.7 g, 6.00 mmol), (see preparation of the silylanion (SiMe$_3$)$_3$Si-K), dropwise via cannula at 0°C. The yellow solutions turns darker and a precipitate was formed. The solution was stirred for 12 h at rt, cooled down again and was added via filter-cannula to a stirred and cooled (0°C) solution of Hyp-K (1.7 g, 6 mmol) in DME. The reactions solution was allowed to warm up to room temperature and stirred for 12 hours. The solid was filtered off and the filtrate was separated into two Schlenk-flasks. One fraction was stored at -30°C for crystallization, the other one was used for further synthesis. All the solvents were removed under reduced pressure and the red-orange, oily residue of ^{t}BuHyp$_2$P was weighted (2.41 g, 4 mmol; yield 70% of the monomer = 1.69 g, 2.9 mmol)) and redissolved in 20 mL of dry DME. KO$_t$Bu (0.39 g, 3.5 mmol) was dissolved in 15

mL dry DME and added drop-wise via syringe at 0°C and was stirred for two hours at rt (NMR for the progress of reaction). The solution was cooled to -30°C and a added dropwise to a stirred solution of $SnBr_2$ (0.40 g,1,44 mmol)in dry THF at -50°C. During the reaction a brown solid formed, the liquid phase was separated from the solid by the use of a syringe. Solvent was removed under reduced pressure until the residue was a yellow, oily liquid, which was stored at -30°C for crystallization. NMR of the solution:
^{31}P NMR (C_6D_6, 293 K): δ -135.62 ppm (no P-Sn coupling constants detected); after 2 weeks storing (303.2 ppm) ^{119}Sn NMR (C_6D_6, 293 K): δ 1592.4 ppm; after 2 weeks storing (1286.32 ppm, $^1J_{Sn\text{-}P}$ = 909.1)

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Bibliography

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Appendix A

Crystallographic data of investigated compounds

Compound	$P(Ph)_2(Si(SiMe_3)_3)$ **3d**	$[Mes^*Si(MeTMS_2)P\text{-}H]$ **4b**	$(Mes^*Hyp)P\text{-}H$ **4c**
Formula	$C_{21}H_{37}PSi_4$	$C_{25}H_{51}PSi_3$	$C_{27}H_{57}PSi_4$
Fw (g mol^{-1})	432.83	466.89	525.05
a (Å)	9.6728(4)	9.9170(7)	23.011(2)
b (Å)	29.9076(13)	11.0333(7)	9.9080(9)
c (Å)	9.1939(4)	15.9245(10)	15.4746(14)
α (°)	90	70.420(2)	90
β (°)	100.394 (1)	77.523(2)	104.904(3)
γ (°)	90	67.152(2)	90
V (Å^3)	2616.06(19)	1505.43(17)	3409.5(5)
Z	4	2	4
Crystal size (mm)	0.12 × 0.10 × 0.09	0.06 × 0.06 × 0.04	0.20 × 0.10 × 0.05
Crystal habit	Block, colourless	Block, colourless	Block, colourless
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	*Cc*	*P*-1	$P2_1/c$
d_{calc} (Mg/m^{-3})	1.099	1.030	1.023
μ (mm^{-1})	0.29	0.22	0.23
T (K)	100(2)	100(2)	100(2)
2*ϑ* range (°)	2.9–33.2	2.4–33.2	2.3–32.7
F(000)	936	516	1160
R_{int}	0.025	0.045	0.098
independent reflns	4577	5234	13067
No. of params	244	282	422
R1, wR2 (all data)[a]	R1 = 0.0209	R1 = 0.3253	R1 = 0.0728
R1, wR2 (>2*σ*)[b]	R1 = 0.0199	R1 = 0.3049	R1 = 0.0462

Compound	Supermesityl-lithiumphosphanide **4e**	Supermesityl-potassiumphosphanide **4f**	Hypersilyl-potassiumphosphanide **5a**	P-Ge cubane **11**
Formula	$C_{46}H_{86}Li_2OP_2Si_2$	$C_{50}H_{96}K_2O_4P_2Si_2$	$C_{37}H_{92}K_2O_4P_2Si_{10}$	$C_{36}H_{108}Ge_4P_4Si_{16}$
Fw (g mol^{-1})	787.14	957.58	962.09	1404.90
a (Å)	12.0851(8)	20.0706(5)	14.0472(17)	21.4062(7)
b (Å)	18.6971(14)	16.8422(4)	13.0421(16)	21.4062(7)
c (Å)	22.1151(16)	18.4115(5)	13.0421(16)	33.6353(12)
α (°)	90	90	90	90
β (°)	93.863(5)	109.1550(12)	104.743(5)	90
γ (°)	90	90	90	90
V (Å^3)	4985.7(6)	5879.1(3)	3043.1(6)	13347.7(10)
Z	4	4	2	6
Crystal size	0.10×0.10×0.08	0.22×0.21×0.17	0.15×0.12×0.09	0.15 × 0.09 ×
Crystal habit	Block, colourless	Block, yellow	Block, orange	Block, red
Crystal	Monoclinic	Monoclinic	Monoclinic	Trigonal
Space group	*I*2/*a*	$P2_1/c$	$P2_1/n$	*R*-3
d_{calc} (mg/m^3)	1.049	1.082	1.050	1.049
μ (mm^{-1})	0.17	0.29	0.43	1.65
T (K)	100(2)	100(2)	100(2)	100(2)
2*ϑ* range (°)	2.7–27.1	2.3–27.2	2.0–27.2	2.5–32.2
F(000)	1736	2096	1048	4416
R_{int}	0.058	0.032	0.48	0.055
independent	5546	13033	5363	11320
No. of	296	668	358	193
R1, wR2 (all	R1 = 0.0457	R1 = 0.0730	R1 = 0.0313	R1 = 0.1065
R1, wR2	R1 = 0.0326	R1 = 0.0655	R1 = 0.0209	R1 = 0.0834

Bond lengths and angles

	P-Si [Å] $_{avg}$	P-C [Å] $_{avg}$	P-H [Å] $_{avg}$	Si-P-C [°] $_{avg}$	C-P-H [°] $_{avg}$	Si-P-H [°] $_{avg}$	C-P-C [°] $_{avg}$
3d	2.281(2)	1.844(2)	—	106.78(4)	—	—	101.21(7)
4b	2.304(3)	1.862(2)	1.25(2)	105.57(4)	102.3(8)	92.7(8)	—
4c	2.321(2)	1.869(2)	1.30(5)	107.69(4)	105(2)	91(2)	—
	Li(1)–O	Li(1) –P	Li(2) –P	P1—Li1—P2	P1—Li2—P2	Li(1)···H–C	
4e	1.908 (3)		2.505 (2) 2.505 (2)	2.412 (2) 2.412 (2)	97.17 (11)	102.32 (12)	
4f	K(1)–O	K(2)–O	K(1) –P	K(2) –P	P1—K1—P2	P1—K2—P2	K(1)···H–C SiMe3 Group (Å)
5a	2.739 (2) 2.821 (2)	2.663 (4) 2.707 (5) 2.782 (5)	3.228 (9) 3.316 (9)	3.205 (9) 3.264 (10)	85.47 (2)	86.71 (2)	2.88 2.92 3.27
	Ge-P [Å] $_{avg}$	P-Si [Å] $_{avg}$	Si-P-Ge [°] $_{avg}$	Ge-P-Gei [°] $_{avg}$	P1-Ge1-P1 [°]		
11	2.459(3)	2.267(3)	120.19(11)	96.81(10)	82.93(13)		

Appendix B

Optimised structures of investigated compounds.

Mes*SnPH_1 E = -2093.48066961 a.u.

0 1

P	1.52786900	-1.43443000	-1.54915800
P	-1.89937700	-2.27596400	0.30067900
Sn	0.33611700	-3.31777400	-0.08302900
C	2.64304500	-0.11968800	-0.72781900
C	3.79224200	-0.41575500	0.07862500
C	2.39351200	1.24375300	-1.11757900
C	4.71786800	0.62005500	0.32334800
C	3.35613100	2.21568300	-0.79818200
C	4.54347900	1.93098300	-0.11805000
H	5.60931100	0.39285000	0.88363900
H	3.18103400	3.23581500	-1.10669100
C	-2.86793800	-0.66478800	0.42693800
C	-2.80647000	0.15883000	1.59659500
C	-3.69863400	-0.28399200	-0.68296100
C	-3.56381500	1.34796700	1.60314300
C	-4.40820400	0.92401200	-0.58469500
C	-4.35866000	1.76080500	0.53480100
H	-3.52769900	1.97459300	2.47842800
H	-5.03179100	1.22462400	-1.41322200
C	1.13366700	1.75119100	-1.88434500
C	1.16123400	1.30657400	-3.36977900
C	-0.16457300	1.29085900	-1.18346900
C	1.04906200	3.29926400	-1.91095600
H	2.08210900	1.65305700	-3.85298800
H	1.10163800	0.22195300	-3.47037600
H	0.30965800	1.74935900	-3.90180500
H	-0.20318200	1.67295800	-0.15799000
H	-1.03620400	1.68078300	-1.72137500
H	-0.26761000	0.20627300	-1.14826700
H	0.09638600	3.58075600	-2.37199000
H	1.07175400	3.73247400	-0.90483000
H	1.84285000	3.75515300	-2.51250200
C	4.08488700	-1.76491300	0.81179900
C	2.96424700	-2.00295500	1.85325000
C	4.25222900	-2.99143700	-0.12480400
C	5.39967500	-1.72118700	1.63608300
H	3.03605100	-1.26890000	2.66304400
H	1.96857800	-1.88000800	1.41349200
H	3.04162100	-3.00709600	2.28659800
H	4.83324500	-2.72932300	-1.01516300
H	4.79005900	-3.78487400	0.40691300

H	3.30349900	-3.41494000	-0.45464100
H	5.49552400	-2.66822000	2.17800800
H	6.28404200	-1.61617600	0.99808400
H	5.40293700	-0.92099300	2.38222200
C	5.56938000	3.04605700	0.13953400
C	4.91359900	4.16609600	0.98339500
C	6.81293400	2.54237100	0.89710200
C	6.03835100	3.63408500	-1.21359700
H	4.04873000	4.60334500	0.47464500
H	4.57354400	3.77611400	1.94890300
H	5.63490500	4.97022700	1.17125000
H	7.33509000	1.75504900	0.34213800
H	7.51596200	3.37077600	1.03766800
H	6.55679100	2.15504500	1.88965500
H	6.75926700	4.44307200	-1.04630300
H	6.52060800	2.86404500	-1.82533700
H	5.20191400	4.04344900	-1.78849700
C	-1.96257400	-0.12344600	2.87856900
C	-2.29401700	-1.50060300	3.50891400
C	-0.45187700	-0.01275300	2.56377400
C	-2.23247500	0.91009700	4.00232000
H	-1.86657900	-1.55065300	4.51726100
H	-3.37735200	-1.64109300	3.59377100
H	-1.88067000	-2.33235000	2.94009200
H	-0.19472600	1.01233200	2.27727900
H	0.13428600	-0.27569800	3.45276100
H	-0.15395700	-0.67483300	1.75096000
H	-1.61208100	0.64575500	4.86500400
H	-1.95830600	1.92970900	3.71273600
H	-3.27735400	0.90256700	4.33172200
C	-3.90487900	-1.10547900	-1.99410300
C	-2.59462500	-1.20056800	-2.81376600
C	-4.47805000	-2.51322800	-1.69038100
C	-4.93623800	-0.44562100	-2.94509600
H	-2.26835600	-0.20413500	-3.12970100
H	-1.77847100	-1.66136500	-2.25801000
H	-2.76823400	-1.80281300	-3.71377100
H	-5.39375300	-2.43472100	-1.09340500
H	-4.72585300	-3.01720300	-2.63226600
H	-3.76783800	-3.14564900	-1.15638100
H	-5.03366800	-1.07834000	-3.83337700
H	-5.92966300	-0.36194000	-2.49079900
H	-4.61627000	0.54389700	-3.28864300
C	-5.16400700	3.06991900	0.55196800
C	-6.67013600	2.75141700	0.38707400
C	-4.98222800	3.85817300	1.86286200
C	-4.70132600	3.97111600	-0.61885000
H	-6.87405200	2.23263700	-0.55474400
H	-7.02517500	2.11545900	1.20512500
H	-7.25486300	3.67873900	0.39330300
H	-3.93591300	4.13906600	2.02604300
H	-5.56974900	4.78174900	1.81858800
H	-5.32745000	3.28772900	2.73225500
H	-5.27882300	4.90289800	-0.62984600
H	-3.64050000	4.22487400	-0.51849600
H	-4.83900800	3.47959300	-1.58692200
H	2.57535400	-2.31525500	-1.97702800
H	-2.63373500	-3.20494000	1.09245700

Mes*SnPH_2 E = -2093.49224526 a.u.

0 1

P	-1.72142	0.05796	1.53795
P	1.68901	0.37863	0.55962
Sn	-0.40502	0.15971	-0.79199
C	-3.44009	0.46899	0.84161

C	-4.34259	-0.48856	0.27176
C	-3.808	1.86156	0.84774
C	-5.49012	-0.01087	-0.39376
C	-4.96805	2.24506	0.15501
C	-5.80973	1.34217	-0.50313
H	-6.15589	-0.72598	-0.84828
H	-5.23335	3.29169	0.12801
C	2.10385	1.27587	2.15926
C	2.38977	2.67993	2.17482
C	2.18775	0.51323	3.37528
C	2.79027	3.25828	3.39696
C	2.58351	1.1811	4.54573
C	2.90054	2.54251	4.58825
H	3.02407	4.30929	3.41569
H	2.65582	0.61684	5.4634
C	-3.04917	2.99096	1.61645
C	-3.00487	2.66566	3.13187
C	-1.61814	3.24284	1.07155
C	-3.77316	4.35704	1.50546
H	-4.02233	2.59179	3.53172
H	-2.48279	1.7299	3.33873
H	-2.48403	3.46898	3.66722
H	-1.62765	3.33519	-0.02163
H	-1.23144	4.18382	1.48078
H	-0.91573	2.45893	1.35981
H	-3.22739	5.08513	2.11456
H	-3.79149	4.73919	0.47858
H	-4.79833	4.31574	1.88797
C	-4.20173	-2.04083	0.36418
C	-3.00482	-2.58413	-0.46118
C	-4.14979	-2.49124	1.84859
C	-5.43477	-2.78122	-0.22005
H	-3.07193	-2.22934	-1.49647
H	-2.02873	-2.30187	-0.06344
H	-3.03848	-3.67992	-0.47972
H	-5.11336	-2.28312	2.32694
H	-3.96865	-3.57144	1.9062
H	-3.38248	-1.99087	2.43909
H	-5.30434	-3.85491	-0.04598
H	-6.36728	-2.48152	0.26845
H	-5.53841	-2.63652	-1.30085
C	-7.03884	1.85505	-1.27049
C	-6.57843	2.82853	-2.38276
C	-7.8381	0.71722	-1.93384
C	-7.98365	2.60261	-0.2982
H	-6.03101	3.68236	-1.9715
H	-5.92064	2.32023	-3.09609
H	-7.4452	3.2172	-2.93063
H	-8.2358	0.01385	-1.19392
H	-8.68887	1.13891	-2.48036
H	-7.22736	0.1575	-2.65085
H	-8.86428	2.97409	-0.83559
H	-8.32408	1.93658	0.50196
H	-7.48906	3.46088	0.16749
C	2.25326	3.66196	0.9679
C	3.61399	4.21277	0.46852
C	1.48516	2.96326	-0.18164
C	1.41616	4.91878	1.32359
H	4.23813	4.53659	1.30873
H	4.17428	3.48267	-0.11417
H	3.4388	5.0824	-0.17562
H	0.47026	2.705	0.14016
H	1.41121	3.63468	-1.0458
H	1.97996	2.04589	-0.50509
H	1.3634	5.55686	0.43533
H	0.38625	4.67519	1.60314

H	1.87303	5.50754	2.12672
C	1.86748	-1.00677	3.51953
C	0.37688	-1.28096	3.20022
C	2.80003	-1.87914	2.64129
C	2.07891	-1.51827	4.96761
H	-0.26876	-0.69449	3.86358
H	0.12415	-1.03723	2.16843
H	0.15391	-2.34323	3.35652
H	3.85024	-1.67157	2.87588
H	2.608	-2.93917	2.84648
H	2.64412	-1.71464	1.57419
H	1.83193	-2.58473	4.99278
H	3.11872	-1.41638	5.29674
H	1.42531	-1.017	5.68973
C	3.34395	3.18647	5.91175
C	4.63087	2.48815	6.41493
C	3.64076	4.69103	5.76703
C	2.22425	3.01723	6.96738
H	4.47253	1.41785	6.57952
H	5.44334	2.60001	5.68895
H	4.95467	2.93018	7.36445
H	2.75643	5.25089	5.44305
H	3.95217	5.09647	6.73585
H	4.45083	4.87895	5.05382
H	2.52943	3.46945	7.91837
H	1.30073	3.50413	6.63605
H	1.99945	1.96275	7.15507
H	-1.28749	1.33641	2.00083
H	2.86989	0.7626	-0.13652

Mes*SnPH_3 E = -2093.49233319 a.u.

0 1

P	-1.2355	0.53385	-0.79558
P	1.79665	-0.0794	1.656
Sn	-0.70501	-0.21493	1.6533
C	-2.97053	1.2912	-0.54501
C	-2.14456	3.1851	-0.52889
C	-3.92148	1.56838	0.06003
C	-2.89965	4.18138	0.12869
C	-4.60569	2.62062	0.68759
C	-4.09798	3.92241	0.78972
H	-2.52991	5.19409	0.12157
H	-5.57499	2.42219	1.12093
C	3.33051	0.18273	2.72333
C	3.83898	1.50292	2.95797
C	4.07196	-0.95849	3.18723
C	5.12906	1.62609	3.51331
C	5.3463	-0.73634	3.73532
C	5.91486	0.5336	3.87964
H	5.53207	2.61402	3.66361
H	5.92257	-1.58878	4.06274
C	-4.71914	0.24434	-0.12779
C	-4.90331	0.01898	-1.65089
C	-4.07663	-0.98146	0.55761
C	-6.15298	0.31732	0.45611
H	-5.57087	0.786	-2.05903
H	-3.96328	0.08463	-2.19466
H	-5.35298	-0.9631	-1.84303
H	-3.98159	-0.80604	1.63629
H	-4.71802	-1.86016	0.41865
H	-3.09123	-1.22489	0.16395
H	-6.66486	-0.62436	0.22846
H	-6.15395	0.43583	1.54536
H	-6.7436	1.12411	0.01096
C	-0.89207	3.69408	-1.31625

C	0.43379	3.42	-0.5613
C	-0.84495	3.0893	-2.74171
C	-0.94471	5.23046	-1.53525
H	0.38288	3.81414	0.46058
H	0.65546	2.35336	-0.51649
H	1.26157	3.92323	-1.07698
H	-1.76982	3.31431	-3.28502
H	-0.00626	3.52656	-3.2969
H	-0.70087	2.00793	-2.72332
H	-0.12988	5.50838	-2.21231
H	-1.886	5.54906	-1.99586
H	-0.79462	5.79635	-0.60963
C	-4.88267	4.99617	1.55947
C	-5.06545	4.53911	3.02724
C	-4.16249	6.35817	1.56884
C	-6.27422	5.19181	0.90948
H	-5.60437	3.58855	3.09051
H	-4.09461	4.40784	3.51698
H	-5.63639	5.28791	3.58884
H	-4.04621	6.76493	0.5582
H	-4.74955	7.0787	2.14897
H	-3.17122	6.28833	2.02999
H	-6.84288	5.95426	1.45491
H	-6.1751	5.51664	-0.13192
H	-6.85987	4.26703	0.91884
C	3.06416	2.83519	2.71415
C	3.86375	4.07808	3.17933
C	2.73694	3.08793	1.22224
C	1.7655	2.83323	3.55419
H	4.12264	4.03467	4.24235
H	4.77902	4.22956	2.59651
H	3.23515	4.9629	3.03317
H	1.98738	2.39098	0.84636
H	2.33563	4.10181	1.10566
H	3.64043	3.01027	0.60711
H	1.21423	3.76729	3.39167
H	1.1131	2.00323	3.28094
H	2.0004	2.75304	4.62136
C	3.56261	-2.43186	3.18455
C	2.2525	-2.53408	4.00138
C	3.35556	-2.98909	1.75464
C	4.56025	-3.39984	3.86871
H	2.42278	-2.22229	5.03827
H	1.45201	-1.92119	3.58465
H	1.89921	-3.57208	4.01329
H	4.25551	-2.84353	1.14621
H	3.15378	-4.06545	1.80867
H	2.50724	-2.51861	1.25613
H	4.10983	-4.39773	3.88748
H	5.50705	-3.48061	3.32296
H	4.77027	-3.11745	4.90588
C	7.33316	0.67873	4.45438
C	8.33157	-0.09186	3.55662
C	7.79223	2.14737	4.52918
C	7.37265	0.08857	5.88522
H	8.07862	-1.15453	3.48835
H	8.33788	0.31759	2.5407
H	9.34588	-0.01345	3.96529
H	7.15271	2.74075	5.19197
H	8.81186	2.19173	4.92717
H	7.80087	2.62074	3.54114
H	8.38013	0.18478	6.30657
H	6.67288	0.61566	6.54264
H	7.10623	-0.97297	5.89331
H	2.29533	-0.52135	0.48191
H	-0.50633	-0.01603	-1.78978

Mes*SnPH_4 E = -2093.49237306 a.u.

0 1

P	-1.72141500	0.05796100	1.53795200
P	1.68900900	0.37862500	0.55962000
Sn	-0.40501500	0.15970600	-0.79198800
C	-3.46660500	-0.08659600	0.80236600
C	-4.07942900	-1.31374400	0.38440400
C	-4.17560100	1.15220500	0.60907700
C	-5.29022700	-1.24441100	-0.33468500
C	-5.37381000	1.12439000	-0.12317500
C	-5.93905500	-0.04752600	-0.63688400
H	-5.73907900	-2.16287700	-0.67553000
H	-5.89488400	2.05381100	-0.29980800
C	3.51002900	0.12113200	0.16772800
C	4.09409500	-1.18737800	0.16071300
C	4.33317800	1.27537900	-0.07203700
C	5.48585100	-1.28768100	-0.04295600
C	5.70780800	1.07302300	-0.27718500
C	6.31407400	-0.18706100	-0.25818400
H	5.93734100	-2.26528400	-0.03291300
H	6.33638200	1.93329400	-0.45205900
C	-3.75117700	2.53533200	1.19992500
C	-3.67102200	2.45112900	2.74612800
C	-2.41520100	3.06387400	0.61340000
C	-4.79424300	3.64127000	0.89729600
H	-4.64795000	2.17773300	3.16016700
H	-2.93513900	1.71885800	3.08267700
H	-3.38707400	3.42848100	3.15523800
H	-2.41523900	2.99423700	-0.48150100
H	-2.29209100	4.12070200	0.87876000
H	-1.54588900	2.53442100	1.00707000
H	-4.46932000	4.56351800	1.39010100
H	-4.87826900	3.85596300	-0.17400700
H	-5.78636800	3.39458600	1.28951300
C	-3.55241100	-2.74919000	0.70011100
C	-2.23281500	-3.08077200	-0.04668800
C	-3.43221700	-2.95549900	2.23374300
C	-4.53946200	-3.85504400	0.23890300
H	-2.35681800	-2.90588800	-1.12197500
H	-1.37249100	-2.50516500	0.29844900
H	-1.98697100	-4.13998700	0.09428300
H	-4.43088600	-2.93429200	2.68409700
H	-2.98491400	-3.93414800	2.44616800
H	-2.83479500	-2.19714900	2.73951700
H	-4.14630300	-4.82384000	0.56599100
H	-5.53160900	-3.73688600	0.68577400
H	-4.64415300	-3.89687700	-0.85064000
C	-7.23460900	0.02014700	-1.46123000
C	-7.00315000	0.91040500	-2.70648300
C	-7.69912500	-1.36636500	-1.94630800
C	-8.36663400	0.63231900	-0.60062300
H	-6.70261500	1.92517700	-2.42768300
H	-6.21702600	0.49065100	-3.34344100
H	-7.92342300	0.98297800	-3.29838500
H	-7.92735400	-2.03527100	-1.10913300
H	-8.61233700	-1.25793100	-2.54179200
H	-6.94534200	-1.84783000	-2.57907600
H	-9.29625900	0.68641100	-1.17955100
H	-8.55074800	0.02231500	0.29030200
H	-8.11991900	1.64560600	-0.26821300
C	3.32721300	-2.54004300	0.30857100
C	2.47725400	-2.62484600	1.60268600
C	2.44851800	-2.77487900	-0.94535900
C	4.28754200	-3.75656300	0.37707900

H	3.04812200	-2.27606900	2.47035300
H	1.55801000	-2.04382500	1.54025000
H	2.19447100	-3.66857400	1.78306100
H	3.07551200	-2.85595700	-1.84011600
H	1.88204800	-3.70784700	-0.83706500
H	1.73787000	-1.96200600	-1.10420800
H	3.68306800	-4.66378700	0.47948700
H	4.88691600	-3.87333500	-0.53138600
H	4.95831700	-3.70705000	1.24194100
C	3.83327200	2.75183400	-0.13481200
C	2.85082000	2.94335600	-1.31682500
C	3.19635600	3.20312200	1.20409800
C	4.98763400	3.75392800	-0.39276700
H	3.33315700	2.66760900	-2.26135900
H	1.94683100	2.34520800	-1.20327400
H	2.54895800	3.99566000	-1.38079500
H	3.90134900	3.05837600	2.03059200
H	2.94969500	4.27027100	1.14939800
H	2.27736900	2.66192900	1.43352500
H	4.56296700	4.76256800	-0.42841700
H	5.73463900	3.74261300	0.40834400
H	5.48918300	3.57928300	-1.35082200
C	7.83098200	-0.31242700	-0.47322200
C	8.57191100	0.47448800	0.63529100
C	8.31572600	-1.77386100	-0.42869800
C	8.20555700	0.27588600	-1.85535400
H	8.30152700	1.53493900	0.62835500
H	8.33057700	0.07253700	1.62516700
H	9.65614300	0.40287700	0.48987600
H	7.85080800	-2.38084000	-1.21348000
H	9.39941500	-1.80391300	-0.58581600
H	8.10868600	-2.24163300	0.54007400
H	9.28653500	0.19603900	-2.02010500
H	7.69456600	-0.26462100	-2.65939400
H	7.93211000	1.33261900	-1.93424100
H	-1.43381500	-1.31474800	1.80238600
H	1.57720000	0.16627800	1.96280700

Mes*SnPH_5 E = -2093.49746508 a.u.

0 1

P	-1.72142	0.05796	1.53795
P	1.68901	0.37863	0.55962
Sn	-0.40502	0.15971	-0.79199
C	-2.61171	1.72679	1.36457
C	-3.84382	1.92757	0.65907
C	-1.94331	2.863	1.94501
C	-4.27663	3.25047	0.43428
C	-2.44529	4.14415	1.66329
C	-3.58534	4.37425	0.88604
H	-5.18721	3.40624	-0.12053
H	-1.93084	5.00297	2.06863
C	3.26758	-0.63762	0.66625
C	3.3315	-1.83721	1.44744
C	4.44268	-0.15819	-0.0095
C	4.57806	-2.48718	1.55776
C	5.63593	-0.88147	0.15075
C	5.7395	-2.03699	0.93163
H	4.64064	-3.38	2.1566
H	6.52594	-0.52704	-0.34725
C	-0.72486	2.79033	2.92091
C	-1.09894	1.96332	4.17804
C	0.55544	2.2198	2.25493
C	-0.31942	4.18994	3.4495
H	-1.93993	2.43183	4.70127
H	-1.37377	0.93653	3.93068

H	-0.24464	1.92854	4.86519
H	0.74585	2.71002	1.29208
H	1.42019	2.41105	2.90152
H	0.50423	1.1401	2.10449
H	0.49328	4.06167	4.17202
H	0.05143	4.84666	2.6545
H	-1.14197	4.69122	3.97019
C	-4.79745	0.80016	0.15167
C	-4.18843	-0.01853	-1.01787
C	-5.24633	-0.10034	1.33346
C	-6.1226	1.36432	-0.42764
H	-3.87052	0.65605	-1.82166
H	-3.33595	-0.63544	-0.72925
H	-4.94831	-0.69405	-1.42837
H	-5.86793	0.48354	2.02143
H	-5.84852	-0.93712	0.95913
H	-4.42309	-0.51406	1.91564
H	-6.77178	0.51996	-0.68403
H	-6.66116	1.98267	0.29735
H	-5.96711	1.94553	-1.34297
C	-4.04135	5.81316	0.59591
C	-2.91282	6.56759	-0.14844
C	-5.30798	5.86617	-0.27949
C	-4.34723	6.53986	1.92828
H	-1.98981	6.59595	0.43898
H	-2.68718	6.08362	-1.10487
H	-3.21541	7.60229	-0.34933
H	-6.16292	5.38873	0.21196
H	-5.57683	6.91103	-0.47002
H	-5.1508	5.38158	-1.24947
H	-4.67279	7.56857	1.73321
H	-5.14272	6.02527	2.47795
H	-3.46648	6.5848	2.57664
C	2.13151	-2.53789	2.16071
C	2.22372	-2.48805	3.70776
C	0.80218	-1.91474	1.66658
C	2.03869	-4.04657	1.81123
H	3.2311	-2.75067	4.04922
H	1.9681	-1.50959	4.11243
H	1.52293	-3.21402	4.13638
H	0.67985	-2.08186	0.59076
H	-0.04542	-2.37933	2.18502
H	0.76324	-0.83917	1.84724
H	1.17984	-4.46845	2.34351
H	1.87105	-4.22348	0.74409
H	2.92884	-4.60109	2.12825
C	4.5149	1.10372	-0.9239
C	3.61255	0.92451	-2.16997
C	4.1552	2.39805	-0.15103
C	5.94126	1.34688	-1.48034
H	3.91257	0.03313	-2.73234
H	2.55936	0.82828	-1.90655
H	3.71364	1.79529	-2.82883
H	4.79895	2.50909	0.72893
H	4.31349	3.26703	-0.80101
H	3.11471	2.41427	0.17636
H	5.91368	2.24049	-2.11255
H	6.67158	1.53223	-0.68522
H	6.29544	0.51913	-2.10429
C	7.09263	-2.75387	1.06614
C	8.12465	-1.7857	1.69431
C	7.0109	-4.00931	1.95492
C	7.58654	-3.18881	-0.33514
H	8.26083	-0.88769	1.08379
H	7.80304	-1.46826	2.69204
H	9.09882	-2.27975	1.78784

H	6.31745	-4.75268	1.54629
H	7.99918	-4.47779	2.01664
H	6.69603	-3.76527	2.97546
H	8.5537	-3.69874	-0.2539
H	6.87361	-3.87662	-0.80247
H	7.71491	-2.33228	-1.00413
H	-0.67895	0.64713	2.31455
H	1.61909	-0.01193	1.92677

Mes*SnPMe_1 E = -2172.08728222 a.u.

0 1

P	-1.72887	-0.71687	1.50017
P	1.73348	0.72703	1.49853
Sn	-0.0037	0.01966	-0.36703
C	-3.3702	-0.29011	0.65107
C	-4.07829	-1.38202	0.04494
C	-3.9023	1.0414	0.53935
C	-5.21908	-1.09394	-0.73046
C	-5.05479	1.22955	-0.24253
C	-5.71882	0.19455	-0.9097
H	-5.73666	-1.90897	-1.20856
H	-5.4537	2.22719	-0.34715
C	3.36651	0.27056	0.64723
C	3.87254	-1.06608	0.53358
C	4.10175	1.3552	0.04977
C	5.03792	-1.27593	-0.23251
C	5.24564	1.04744	-0.70411
C	5.72981	-0.25263	-0.87897
H	5.41325	-2.28002	-0.33614
H	5.7898	1.85357	-1.173
C	-3.34351	2.31393	1.25338
C	-3.47622	2.16676	2.7926
C	-1.88615	2.66151	0.8358
C	-4.15938	3.58776	0.90557
H	-4.5355	2.13459	3.07017
H	-3.00903	1.2629	3.18548
H	-3.01819	3.02811	3.29344
H	-1.75335	2.50697	-0.2452
H	-1.68576	3.72066	1.03321
H	-1.12837	2.10038	1.38422
H	-3.74454	4.4266	1.47411
H	-4.09657	3.84586	-0.15736
H	-5.21263	3.49804	1.18822
C	-3.71307	-2.89322	0.19895
C	-2.33355	-3.23452	-0.42347
C	-3.76395	-3.31315	1.69057
C	-4.72393	-3.81894	-0.52515
H	-2.25737	-2.83334	-1.44101
H	-1.50464	-2.8519	0.17398
H	-2.21608	-4.32339	-0.48042
H	-4.77341	-3.16363	2.08959
H	-3.51361	-4.37723	1.78322
H	-3.06116	-2.74705	2.30391
H	-4.43457	-4.85762	-0.33337
H	-5.74552	-3.6922	-0.15203
H	-4.72158	-3.67467	-1.61134
C	-6.95458	0.5018	-1.77072
C	-6.5697	1.50288	-2.88713
C	-7.53486	-0.759	-2.43972
C	-8.0587	1.12707	-0.8834
H	-6.18679	2.44191	-2.47538
H	-5.79598	1.08088	-3.5376
H	-7.44551	1.73927	-3.50295
H	-7.87454	-1.49236	-1.70002
H	-8.39977	-0.48265	-3.05268

H	-6.80325	-1.24288	-3.0962
H	-8.94689	1.3536	-1.48504
H	-8.35122	0.43778	-0.08401
H	-7.72296	2.05865	-0.41694
C	3.27514	-2.33379	1.22539
C	3.41236	-2.21549	2.76698
C	1.80598	-2.62791	0.8053
C	4.05175	-3.62625	0.85602
H	4.47207	-2.21902	3.04462
H	2.97191	-1.30406	3.17352
H	2.92896	-3.07058	3.25458
H	1.66092	-2.39587	-0.26122
H	1.58932	-3.69512	0.92721
H	1.06524	-2.09597	1.40366
H	3.60522	-4.46271	1.40376
H	3.9893	-3.85915	-0.21265
H	5.10513	-3.57842	1.14797
C	3.75659	2.87132	0.19839
C	2.38352	3.22843	-0.42893
C	3.8091	3.29509	1.68887
C	4.78174	3.78014	-0.52668
H	2.30535	2.82719	-1.44624
H	1.54828	2.85645	0.16641
H	2.27898	4.31849	-0.487
H	4.8146	3.13051	2.09192
H	3.5756	4.36333	1.77737
H	3.09511	2.74216	2.30132
H	4.50243	4.82351	-0.34617
H	5.79933	3.64616	-0.14508
H	4.78489	3.62571	-1.61154
C	6.98166	-0.49774	-1.73732
C	8.17944	0.28035	-1.13984
C	7.36697	-1.98768	-1.80736
C	6.72028	-0.00074	-3.18012
H	7.98778	1.35747	-1.1075
H	8.38929	-0.05389	-0.11809
H	9.07786	0.11777	-1.74694
H	6.5678	-2.59331	-2.2489
H	8.25741	-2.10581	-2.43454
H	7.60307	-2.39367	-0.81749
H	7.61063	-0.15486	-3.80121
H	5.88561	-0.54572	-3.63412
H	6.47611	1.06589	-3.20167
C	-1.51197	0.70527	2.61501
H	-1.78432	1.60454	2.10311
H	-2.13549	0.58204	3.47578
H	-0.48859	0.76533	2.92156
C	1.49528	-0.69628	2.60751
H	1.74735	-1.59804	2.08964
H	2.12583	-0.58947	3.46537
H	0.47264	-0.73811	2.91952

Mes*SnPMe_2 E = -2172.08868003 a.u.

0 1

P	1.52787	-1.43443	-1.54916
P	-1.89938	-2.27596	0.30068
Sn	0.33612	-3.31777	-0.08303
C	2.64305	-0.11969	-0.72782
C	3.79224	-0.41576	0.07863
C	2.39351	1.24375	-1.11758
C	4.71787	0.62006	0.32335
C	3.35613	2.21568	-0.79818
C	4.54348	1.93098	-0.11805
H	5.60931	0.39285	0.88364
H	3.18103	3.23582	-1.10669

C	-2.86794	-0.66479	0.42694
C	-2.80647	0.15883	1.5966
C	-3.69863	-0.28399	-0.68296
C	-3.56382	1.34797	1.60314
C	-4.4082	0.92401	-0.5847
C	-4.35866	1.76081	0.5348
H	-3.5277	1.97459	2.47843
H	-5.03179	1.22462	-1.41322
C	1.13367	1.75119	-1.88435
C	1.16123	1.30657	-3.36978
C	-0.16457	1.29086	-1.18347
C	1.04906	3.29926	-1.91096
H	2.08211	1.65306	-3.85299
H	1.10164	0.22195	-3.47038
H	0.30966	1.74936	-3.90181
H	-0.20318	1.67296	-0.15799
H	-1.0362	1.68078	-1.72138
H	-0.26761	0.20627	-1.14827
H	0.09639	3.58076	-2.37199
H	1.07175	3.73247	-0.90483
H	1.84285	3.75515	-2.5125
C	4.08489	-1.76491	0.8118
C	2.96425	-2.00296	1.85325
C	4.25223	-2.99144	-0.1248
C	5.39968	-1.72119	1.63608
H	3.03605	-1.2689	2.66304
H	1.96858	-1.88001	1.41349
H	3.04162	-3.0071	2.2866
H	4.83325	-2.72932	-1.01516
H	4.79006	-3.78487	0.40691
H	3.3035	-3.41494	-0.45464
H	5.49552	-2.66822	2.17801
H	6.28404	-1.61618	0.99808
H	5.40294	-0.92099	2.38222
C	5.56938	3.04606	0.13953
C	4.9136	4.1661	0.9834
C	6.81293	2.54237	0.8971
C	6.03835	3.63409	-1.2136
H	4.04873	4.60335	0.47465
H	4.57354	3.77611	1.9489
H	5.6349	4.97023	1.17125
H	7.33509	1.75505	0.34214
H	7.51596	3.37078	1.03767
H	6.55679	2.15504	1.88966
H	6.75927	4.44307	-1.0463
H	6.52061	2.86405	-1.82534
H	5.20191	4.04345	-1.7885
C	-1.96257	-0.12345	2.87857
C	-2.29402	-1.5006	3.50891
C	-0.45188	-0.01275	2.56377
C	-2.23247	0.9101	4.00232
H	-1.86658	-1.55065	4.51726
H	-3.37735	-1.64109	3.59377
H	-1.88067	-2.33235	2.94009
H	-0.19473	1.01233	2.27728
H	0.13429	-0.2757	3.45276
H	-0.15396	-0.67483	1.75096
H	-1.61208	0.64576	4.865
H	-1.95831	1.92971	3.71274
H	-3.27735	0.90257	4.33172
C	-3.90488	-1.10548	-1.9941
C	-2.59463	-1.20057	-2.81377
C	-4.47805	-2.51323	-1.69038
C	-4.93624	-0.44562	-2.9451
H	-2.26836	-0.20414	-3.1297
H	-1.77847	-1.66137	-2.25801

H	-2.76823	-1.80281	-3.71377
H	-5.39375	-2.43472	-1.0934
H	-4.72585	-3.0172	-2.63227
H	-3.76784	-3.14565	-1.15638
H	-5.03367	-1.07834	-3.83338
H	-5.92966	-0.36194	-2.4908
H	-4.61627	0.5439	-3.28864
C	-5.16401	3.06992	0.55197
C	-6.67014	2.75142	0.38707
C	-4.98223	3.85817	1.86286
C	-4.70133	3.97112	-0.61885
H	-6.87405	2.23264	-0.55474
H	-7.02517	2.11546	1.20513
H	-7.25486	3.67874	0.3933
H	-3.93591	4.13907	2.02604
H	-5.56975	4.78175	1.81859
H	-5.32745	3.28773	2.73226
H	-5.27882	4.9029	-0.62985
H	-3.6405	4.22487	-0.5185
H	-4.83901	3.47959	-1.58692
C	-2.83763	-3.46286	1.31229
H	-3.05544	-4.3338	0.73011
H	-2.25649	-3.74106	2.16657
H	-3.75256	-3.01153	1.63493
C	2.85738	-2.55241	-2.09223
H	3.80446	-2.07427	-1.95325
H	2.82428	-3.45278	-1.51504
H	2.72503	-2.78746	-3.12767

Mes*SnPMe_3 E = -2172.09148100 a.u.

0 1

P	-1.72142	0.05796	1.53795
P	1.68901	0.37863	0.55962
Sn	-0.40502	0.15971	-0.79199
C	-3.46661	-0.0866	0.80237
C	-4.07943	-1.31374	0.3844
C	-4.1756	1.15221	0.60908
C	-5.29023	-1.24441	-0.33469
C	-5.37381	1.12439	-0.12318
C	-5.93906	-0.04753	-0.63688
H	-5.73908	-2.16288	-0.67553
H	-5.89488	2.05381	-0.29981
C	3.51003	0.12113	0.16773
C	4.0941	-1.18738	0.16071
C	4.33318	1.27538	-0.07204
C	5.48585	-1.28768	-0.04296
C	5.70781	1.07302	-0.27719
C	6.31407	-0.18706	-0.25818
H	5.93734	-2.26528	-0.03291
H	6.33638	1.93329	-0.45206
C	-3.75118	2.53533	1.19993
C	-3.67102	2.45113	2.74613
C	-2.4152	3.06387	0.6134
C	-4.79424	3.64127	0.8973
H	-4.64795	2.17773	3.16017
H	-2.93514	1.71886	3.08268
H	-3.38707	3.42848	3.15524
H	-2.41524	2.99424	-0.4815
H	-2.29209	4.1207	0.87876
H	-1.54589	2.53442	1.00707
H	-4.46932	4.56352	1.3901
H	-4.87827	3.85596	-0.17401
H	-5.78637	3.39459	1.28951
C	-3.55241	-2.74919	0.70011
C	-2.23281	-3.08077	-0.04669

C	-3.43222	-2.9555	2.23374
C	-4.53946	-3.85504	0.2389
H	-2.35682	-2.90589	-1.12198
H	-1.37249	-2.50517	0.29845
H	-1.98697	-4.13999	0.09428
H	-4.43089	-2.93429	2.6841
H	-2.98491	-3.93415	2.44617
H	-2.8348	-2.19715	2.73952
H	-4.1463	-4.82384	0.56599
H	-5.53161	-3.73689	0.68577
H	-4.64415	-3.89688	-0.85064
C	-7.23461	0.02015	-1.46123
C	-7.00315	0.91041	-2.70648
C	-7.69913	-1.36637	-1.94631
C	-8.36663	0.63232	-0.60062
H	-6.70262	1.92518	-2.42768
H	-6.21703	0.49065	-3.34344
H	-7.92342	0.98298	-3.29839
H	-7.92735	-2.03527	-1.10913
H	-8.61234	-1.25793	-2.54179
H	-6.94534	-1.84783	-2.57908
H	-9.29626	0.68641	-1.17955
H	-8.55075	0.02232	0.2903
H	-8.11992	1.64561	-0.26821
C	3.32721	-2.54004	0.30857
C	2.47725	-2.62485	1.60269
C	2.44852	-2.77488	-0.94536
C	4.28754	-3.75656	0.37708
H	3.04812	-2.27607	2.47035
H	1.55801	-2.04383	1.54025
H	2.19447	-3.66857	1.78306
H	3.07551	-2.85596	-1.84012
H	1.88205	-3.70785	-0.83707
H	1.73787	-1.96201	-1.10421
H	3.68307	-4.66379	0.47949
H	4.88692	-3.87334	-0.53139
H	4.95832	-3.70705	1.24194
C	3.83327	2.75183	-0.13481
C	2.85082	2.94336	-1.31683
C	3.19636	3.20312	1.2041
C	4.98763	3.75393	-0.39277
H	3.33316	2.66761	-2.26136
H	1.94683	2.34521	-1.20327
H	2.54896	3.99566	-1.3808
H	3.90135	3.05838	2.03059
H	2.9497	4.27027	1.1494
H	2.27737	2.66193	1.43353
H	4.56297	4.76257	-0.42842
H	5.73464	3.74261	0.40834
H	5.48918	3.57928	-1.35082
C	7.83098	-0.31243	-0.47322
C	8.57191	0.47449	0.63529
C	8.31573	-1.77386	-0.4287
C	8.20556	0.27589	-1.85535
H	8.30153	1.53494	0.62836
H	8.33058	0.07254	1.62517
H	9.65614	0.40288	0.48988
H	7.85081	-2.38084	-1.21348
H	9.39941	-1.80391	-0.58582
H	8.10869	-2.24163	0.54007
H	9.28654	0.19604	-2.02011
H	7.69457	-0.26462	-2.65939
H	7.93211	1.33262	-1.93424
C	-1.35467	-1.69252	1.87516
H	-0.35997	-1.91735	1.55123
H	-1.43831	-1.87854	2.92554

H	-2.0501	-2.31081	1.34696
C	1.54606	0.10714	2.35357
H	1.08318	0.95845	2.80736
H	0.95016	-0.76257	2.53632
H	2.5208	-0.03405	2.77172

Mes*SnPMe_4 E = -2172.09161276 a.u.

0 1

P	-1.08746	0.21723	-0.82885
P	1.81346	0.05822	1.72545
Sn	-0.67881	0.08169	1.80982
C	-2.97904	0.02796	-0.75763
C	-3.73405	1.24809	-0.67817
C	-3.681	-1.22802	-0.7442
C	-5.12072	1.16546	-0.43834
C	-5.06728	-1.21142	-0.51592
C	-5.80926	-0.04105	-0.3237
H	-5.68179	2.08018	-0.34293
H	-5.59654	-2.15232	-0.48275
C	3.36751	-0.00445	0.65674
C	3.97348	-1.26151	0.33642
C	3.98943	1.22104	0.23977
C	5.21555	-1.24431	-0.33029
C	5.22499	1.13658	-0.42259
C	5.8695	-0.07183	-0.70641
H	5.68771	-2.18505	-0.55978
H	5.70855	2.05231	-0.72788
C	-3.04679	-2.62753	-1.01553
C	-2.38412	-2.65848	-2.41889
C	-2.0753	-3.06479	0.11165
C	-4.10619	-3.76008	-1.06373
H	-3.15962	-2.58663	-3.18963
H	-1.67813	-1.84743	-2.59627
H	-1.85128	-3.60649	-2.56045
H	-2.59397	-3.05023	1.07736
H	-1.73415	-4.09065	-0.07183
H	-1.18506	-2.44125	0.19325
H	-3.59791	-4.69425	-1.3264
H	-4.59615	-3.91686	-0.09666
H	-4.87221	-3.58031	-1.82485
C	-3.15707	2.68498	-0.89421
C	-2.126	3.09596	0.18956
C	-2.53471	2.80252	-2.30988
C	-4.25903	3.77351	-0.83506
H	-2.50797	2.87652	1.19424
H	-1.16092	2.60557	0.05282
H	-1.94365	4.17581	0.13227
H	-3.29644	2.61051	-3.07372
H	-2.14777	3.81801	-2.45981
H	-1.71045	2.10307	-2.45854
H	-3.79518	4.74142	-1.05223
H	-5.04307	3.61459	-1.58258
H	-4.72236	3.84851	0.15516
C	-7.31746	-0.12257	-0.03862
C	-7.55202	-0.9355	1.2578
C	-7.95795	1.26628	0.14562
C	-8.02955	-0.82789	-1.21875
H	-7.15375	-1.95167	1.17548
H	-7.06604	-0.45252	2.1124
H	-8.62526	-1.01116	1.46953
H	-7.86715	1.87894	-0.75807
H	-9.02582	1.15132	0.36171
H	-7.50699	1.81292	0.98114
H	-9.10776	-0.88989	-1.02939
H	-7.87482	-0.27485	-2.15143

H	-7.65631	-1.84621	-1.36637
C	3.37031	-2.66719	0.6363
C	4.27306	-3.81998	0.12869
C	3.20151	-2.91923	2.15575
C	2.02448	-2.83658	-0.10939
H	4.43934	-3.7761	-0.9527
H	5.24329	-3.84607	0.63682
H	3.76809	-4.76813	0.34156
H	2.42341	-2.29771	2.59831
H	2.9241	-3.967	2.32291
H	4.14206	-2.72826	2.68464
H	1.59318	-3.8187	0.11861
H	1.29978	-2.07456	0.17917
H	2.17859	-2.77188	-1.19223
C	3.40257	2.65031	0.43879
C	2.05554	2.77959	-0.3125
C	3.25299	3.01087	1.9384
C	4.31498	3.75254	-0.15614
H	2.20899	2.65942	-1.39058
H	1.32418	2.03544	0.00261
H	1.62519	3.77301	-0.13694
H	4.20608	2.87585	2.46248
H	2.95887	4.06307	2.03342
H	2.49427	2.40872	2.4386
H	3.82193	4.71927	-0.00957
H	5.28904	3.80404	0.34309
H	4.47219	3.62889	-1.23287
C	7.23367	-0.0662	-1.41489
C	8.25483	0.71377	-0.55118
C	7.78604	-1.48574	-1.64367
C	7.09594	0.62516	-2.79313
H	7.93751	1.74762	-0.38345
H	8.38008	0.23773	0.42728
H	9.231	0.7385	-1.04953
H	7.12516	-2.08154	-2.28277
H	8.7596	-1.42318	-2.14186
H	7.93143	-2.02217	-0.69945
H	8.06466	0.64233	-3.30598
H	6.38069	0.09011	-3.42697
H	6.74999	1.65891	-2.69563
C	-0.58215	-1.48679	-1.2205
H	-0.33272	-1.55513	-2.25878
H	0.27081	-1.75036	-0.63068
H	-1.38746	-2.15668	-1.00231
C	2.45769	-0.01455	3.42606
H	2.14684	0.85732	3.96283
H	2.07837	-0.88796	3.91409
H	3.5266	-0.05578	3.40108

Mes*SnPtBu_1 E = -2407.83918599 a.u.

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P	2.10792	-1.41439	0.25259
P	-2.12491	-1.40636	-0.27765
Sn	-0.00659	0.00672	0.00588
C	3.35832	0.01085	0.08693
C	3.76368	0.6778	1.29355
C	3.69838	0.60119	-1.18425
C	4.32054	1.97119	1.18762
C	4.2473	1.89394	-1.18869
C	4.52985	2.6207	-0.02647
H	4.58912	2.49016	2.09318
H	4.46148	2.36122	-2.1382
C	-3.36444	0.02338	-0.06938
C	-3.68651	0.59282	1.21084
C	-3.77567	0.71752	-1.26373

C	-4.21668	1.8983	1.24749
C	-4.31412	2.01033	-1.12655
C	-4.499	2.646	0.10412
H	-4.40697	2.34888	2.20758
H	-4.59198	2.55067	-2.01964
C	3.61972	-0.10918	-2.57268
C	4.52431	-1.36073	-2.51426
C	2.19248	-0.50111	-3.02511
C	4.18558	0.76498	-3.72047
H	5.56545	-1.07232	-2.33119
H	4.2163	-2.0303	-1.71327
H	4.47877	-1.90976	-3.46253
H	1.51504	0.3599	-2.96662
H	2.22209	-0.83299	-4.07057
H	1.77522	-1.30679	-2.4241
H	4.16693	0.17304	-4.64187
H	3.58203	1.66206	-3.89755
H	5.22446	1.06395	-3.547
C	3.67079	0.10774	2.74694
C	2.2295	0.17283	3.31401
C	4.19907	-1.34196	2.81931
C	4.55386	0.91345	3.73762
H	1.80983	1.17874	3.19607
H	1.57385	-0.54253	2.81635
H	2.24656	-0.06379	4.38541
H	5.2294	-1.3998	2.45069
H	4.18534	-1.68722	3.86027
H	3.57678	-2.01659	2.23206
H	4.56416	0.38343	4.696
H	5.58962	0.9986	3.3918
H	4.1629	1.91734	3.93453
C	5.08445	4.05039	-0.12912
C	4.08073	4.93537	-0.90741
C	5.31776	4.69248	1.25165
C	6.4364	4.02737	-0.88358
H	3.896	4.5488	-1.91461
H	3.11897	4.98384	-0.38563
H	4.47163	5.95514	-1.00506
H	6.06083	4.14005	1.83737
H	5.69209	5.71389	1.12177
H	4.39116	4.74938	1.83341
H	6.84349	5.04226	-0.96372
H	7.16576	3.40473	-0.35428
H	6.32758	3.62904	-1.89731
C	-3.60984	-0.14555	2.58468
C	-4.53406	-1.3818	2.50489
C	-2.18673	-0.56896	3.02072
C	-4.15582	0.71294	3.7536
H	-5.57158	-1.07352	2.33393
H	-4.24122	-2.03827	1.68737
H	-4.49226	-1.95201	3.44086
H	-1.49714	0.28349	2.97964
H	-2.21639	-0.92489	4.05823
H	-1.78387	-1.36585	2.39872
H	-4.14226	0.1011	4.66206
H	-3.537	1.59617	3.94651
H	-5.19025	1.03281	3.59185
C	-3.70438	0.1695	-2.72649
C	-2.26815	0.22807	-3.30736
C	-4.24951	-1.27294	-2.81588
C	-4.58865	1.00148	-3.69377
H	-1.83671	1.22767	-3.17841
H	-1.61476	-0.50139	-2.82745
H	-2.29885	0.00818	-4.38202
H	-5.27694	-1.32533	-2.43845
H	-4.24936	-1.6022	-3.86209

H	-3.62922	-1.96343	-2.24509
H	-4.61468	0.48879	-4.66119
H	-5.61977	1.09145	-3.33538
H	-4.18851	2.00446	-3.87692
C	-5.02655	4.0888	0.15559
C	-6.42795	4.15215	-0.49957
C	-5.14614	4.6216	1.59616
C	-4.0585	5.01498	-0.62013
H	-6.40016	3.83182	-1.5457
H	-7.13479	3.50546	0.0315
H	-6.8129	5.17852	-0.47237
H	-4.17957	4.61376	2.11176
H	-5.50411	5.65683	1.57448
H	-5.85925	4.03775	2.18862
H	-4.42591	6.04794	-0.60237
H	-3.05967	4.99702	-0.17105
H	-3.96067	4.71133	-1.66707
C	-4.57727	-3.92161	-0.34421
H	-4.73665	-3.91587	-1.42604
H	-4.87527	-4.90513	0.04053
H	-5.2383	-3.17163	0.09661
C	-2.34962	-4.27236	1.81552
H	-3.05207	-3.88241	2.55615
H	-2.4154	-5.36798	1.82516
H	-1.34045	-3.99094	2.12958
C	-1.68456	-4.58122	-1.19747
H	-0.61597	-4.40897	-1.04601
H	-1.8696	-5.65886	-1.10818
H	-1.93526	-4.27077	-2.21654
C	2.32213	-4.25265	-1.86726
H	1.31471	-3.95893	-2.17564
H	3.02641	-3.85671	-2.60299
H	2.37996	-5.34841	-1.89326
C	1.66097	-4.60155	1.14235
H	0.59263	-4.42598	0.99304
H	1.84452	-5.67826	1.03946
H	1.91211	-4.30465	2.16533
C	4.55443	-3.93806	0.29554
H	4.84786	-4.92026	-0.09607
H	5.21753	-3.18789	-0.14175
H	4.71577	-3.94005	1.37704
C	-2.73989	-3.62888	0.06523
C	2.71768	-3.6356	-0.10874

Mes*SnPtBu_2 E = -2407.84581479 a.u.

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P	2.05038	1.08461	0.47792
P	-1.86042	0.36493	0.28163
Sn	0.32858	-0.4783	-0.66243
C	3.67447	0.17542	0.04348
C	4.11622	-0.12878	-1.28511
C	4.38895	-0.41379	1.16166
C	5.13704	-1.09887	-1.44791
C	5.40458	-1.34213	0.89446
C	5.7791	-1.73611	-0.39625
H	5.43061	-1.36052	-2.454
H	5.92328	-1.79423	1.72598
C	-3.51902	-0.42819	-0.1936
C	-4.34675	0.19333	-1.18813
C	-4.04921	-1.53447	0.56229
C	-5.71571	-0.14602	-1.22371
C	-5.42526	-1.8015	0.46057
C	-6.29292	-1.09246	-0.37758
H	-6.35018	0.35364	-1.93741
H	-5.84168	-2.59804	1.05925

C	4.13863	-0.12225	2.67796
C	4.16549	1.3946	2.97344
C	2.80969	-0.75316	3.16572
C	5.24372	-0.72639	3.58482
H	5.11885	1.83252	2.65522
H	3.34969	1.91048	2.46917
H	4.05412	1.5633	4.05131
H	2.79947	-1.82939	2.95685
H	2.71232	-0.61539	4.25004
H	1.94897	-0.29386	2.67991
H	5.05154	-0.40436	4.6138
H	5.23657	-1.82163	3.58819
H	6.24533	-0.37748	3.31015
C	3.69083	0.45374	-2.67961
C	2.67542	1.60485	-2.72726
C	4.96602	1.04019	-3.35656
C	3.11977	-0.68258	-3.56931
H	1.67541	1.32575	-2.3954
H	3.0046	2.44845	-2.12245
H	2.59643	1.94903	-3.76611
H	5.75348	0.29926	-3.50798
H	4.70475	1.45085	-4.339
H	5.38345	1.84905	-2.74679
H	2.84262	-0.28094	-4.5514
H	3.83567	-1.49297	-3.73081
H	2.22351	-1.11792	-3.11357
C	6.86369	-2.80611	-0.59235
C	6.41209	-4.12242	0.08597
C	7.13755	-3.10372	-2.079
C	8.18629	-2.32628	0.05323
H	6.23828	-3.98611	1.1579
H	5.48202	-4.49042	-0.36042
H	7.18142	-4.8943	-0.03455
H	7.50326	-2.21803	-2.61068
H	7.90723	-3.87905	-2.16101
H	6.2415	-3.47112	-2.59156
H	8.96753	-3.0846	-0.07605
H	8.52957	-1.39544	-0.41089
H	8.07092	-2.14386	1.12613
C	-3.85216	1.16508	-2.3052
C	-3.38167	2.53321	-1.76037
C	-2.72398	0.48201	-3.11546
C	-4.96151	1.48962	-3.33775
H	-4.1832	3.01066	-1.1845
H	-2.50364	2.43429	-1.12269
H	-3.12701	3.19443	-2.59791
H	-3.08678	-0.44711	-3.56874
H	-2.38305	1.14719	-3.91816
H	-1.86339	0.24198	-2.48978
H	-4.52133	2.10367	-4.13087
H	-5.37014	0.58905	-3.80819
H	-5.7843	2.06722	-2.90214
C	-3.2124	-2.55303	1.39912
C	-2.18549	-3.2248	0.45546
C	-2.50201	-1.94282	2.62901
C	-4.07697	-3.70935	1.96236
H	-2.70001	-3.7506	-0.3565
H	-1.50653	-2.49877	0.00495
H	-1.58053	-3.95271	1.00963
H	-3.23232	-1.50251	3.31723
H	-1.96885	-2.7344	3.16979
H	-1.77934	-1.17935	2.3452
H	-3.41321	-4.40973	2.48077
H	-4.81564	-3.36129	2.69315
H	-4.59234	-4.26976	1.17535
C	-7.79687	-1.40847	-0.37373

C	-8.36397	-1.16718	1.04655
C	-8.58619	-0.52764	-1.36053
C	-8.0196	-2.88967	-0.766
H	-7.86483	-1.7935	1.79259
H	-8.23315	-0.12143	1.34495
H	-9.43481	-1.4016	1.0722
H	-8.26661	-0.68953	-2.3959
H	-9.65165	-0.77544	-1.30111
H	-8.47857	0.53751	-1.12768
H	-9.09082	-3.12336	-0.76983
H	-7.61996	-3.09168	-1.76557
H	-7.53085	-3.57261	-0.0641
C	-4.12097	1.5108	2.59877
H	-4.82279	1.58922	1.76279
H	-4.22827	0.51316	3.03028
H	-4.40468	2.24969	3.359
C	-1.07542	1.51543	3.40193
H	-1.2844	0.56514	3.90165
H	-0.05664	1.46663	3.00325
H	-1.11214	2.31309	4.15419
C	-2.23672	3.6667	1.47853
H	-1.3093	3.89542	0.94863
H	-3.07328	3.92846	0.82512
H	-2.28536	4.30955	2.36688
C	1.61427	4.13665	1.95321
H	0.66396	3.72155	2.29698
H	2.36721	3.92958	2.71918
H	1.50177	5.22527	1.87151
C	0.91813	4.06541	-1.049
H	0.68235	5.11863	-0.85288
H	1.32791	3.99045	-2.05932
H	-0.01838	3.49836	-1.02698
C	3.92554	3.98516	-0.05943
H	3.99251	5.07166	0.07952
H	4.61025	3.50932	0.64887
H	4.27268	3.75153	-1.06891
C	-2.34218	1.84525	2.02298
C	2.13679	3.4189	0.26734

Mes*SnPtBu_3 E = -2407.84713045 a.u.

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P	1.62467	-1.21949	0.44957
P	-1.66634	1.19733	-0.48645
Sn	0.84127	0.98961	-0.63693
C	3.48234	-0.78676	0.33516
C	4.05673	-0.209	1.51978
C	4.23875	-0.74277	-0.89099
C	5.23085	0.56404	1.38613
C	5.39193	0.05788	-0.93207
C	5.88451	0.76369	0.17232
H	5.6365	1.03479	2.26698
H	5.93203	0.13942	-1.86409
C	-3.28126	0.3033	-0.04976
C	-4.04822	-0.35305	-1.06895
C	-3.82005	0.40462	1.28118
C	-5.37965	-0.71078	-0.77266
C	-5.15655	0.01913	1.48151
C	-5.97385	-0.4977	0.47051
H	-5.97212	-1.1691	-1.54761
H	-5.58041	0.12694	2.46912
C	3.96663	-1.61729	-2.15218
C	4.04194	-3.09622	-1.70827
C	2.62653	-1.3272	-2.86567
C	5.05375	-1.44702	-3.24255
H	5.04336	-3.32639	-1.32813

H	3.32937	-3.30827	-0.91235
H	3.83224	-3.76357	-2.55293
H	2.55942	-0.26742	-3.14133
H	2.56949	-1.91725	-3.78874
H	1.76558	-1.57934	-2.24976
H	4.83604	-2.14675	-4.05693
H	5.05918	-0.43905	-3.67204
H	6.05692	-1.68003	-2.87136
C	3.51912	-0.36672	2.97942
C	2.30847	0.55926	3.25994
C	3.14958	-1.83595	3.28604
C	4.59876	0.00936	4.02971
H	2.54246	1.59573	2.98881
H	1.42705	0.24056	2.7035
H	2.0695	0.53545	4.33095
H	4.00983	-2.49533	3.1234
H	2.84084	-1.9258	4.33457
H	2.32324	-2.17572	2.66204
H	4.22248	-0.26556	5.02091
H	5.53791	-0.53024	3.86661
H	4.80867	1.08392	4.05768
C	7.11224	1.67533	0.01946
C	6.79287	2.78286	-1.01448
C	7.50894	2.35459	1.34378
C	8.32222	0.84754	-0.47725
H	6.54375	2.36076	-1.9932
H	5.94222	3.38899	-0.68469
H	7.65838	3.4437	-1.1426
H	7.78616	1.62149	2.10932
H	8.376	3.00331	1.17774
H	6.69833	2.97692	1.7384
H	9.20023	1.49376	-0.59412
H	8.57092	0.05569	0.23748
H	8.12262	0.37723	-1.44517
C	-3.52546	-0.76749	-2.47841
C	-4.54715	-1.6312	-3.26006
C	-3.22396	0.44782	-3.38266
C	-2.26512	-1.65053	-2.33022
H	-4.83718	-2.5329	-2.71055
H	-5.45092	-1.07297	-3.5281
H	-4.07704	-1.953	-4.19563
H	-2.39363	1.03237	-2.98918
H	-2.95253	0.10126	-4.38738
H	-4.10497	1.09331	-3.47381
H	-1.88427	-1.92164	-3.32286
H	-1.46779	-1.13612	-1.79103
H	-2.50952	-2.57383	-1.79367
C	-3.03241	0.8503	2.55057
C	-1.7863	-0.0472	2.73147
C	-2.62265	2.33956	2.50826
C	-3.86006	0.67944	3.84912
H	-2.09022	-1.0863	2.89647
H	-1.12279	-0.02021	1.86592
H	-1.21207	0.28416	3.60495
H	-3.49064	2.97803	2.30474
H	-2.2065	2.6333	3.47963
H	-1.86383	2.51958	1.74813
H	-3.21614	0.93149	4.69848
H	-4.72549	1.35076	3.88848
H	-4.20263	-0.35087	3.99242
C	-7.44227	-0.84142	0.76703
C	-8.17658	0.42995	1.25787
C	-8.18555	-1.37156	-0.47383
C	-7.50929	-1.92636	1.86939
H	-7.71942	0.83806	2.16478
H	-8.15598	1.21147	0.49069

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H	-9.22389	0.19807	1.4848
H	-7.74902	-2.30623	-0.843
H	-9.23041	-1.57521	-0.21501
H	-8.18117	-0.64123	-1.29042
H	-8.55368	-2.17466	2.09294
H	-6.99974	-2.84065	1.54665
H	-7.03848	-1.58908	2.79804
C	1.8991	-4.60741	1.13811
H	1.77987	-4.45533	2.21472
H	1.5966	-5.63563	0.90261
H	2.96093	-4.50439	0.90016
C	0.54376	-4.03824	-1.60818
H	0.02652	-5.00535	-1.55159
H	-0.07912	-3.35816	-2.1944
H	1.48579	-4.18766	-2.13915
C	-0.89808	-3.29386	1.01693
H	-0.77778	-3.06528	2.07966
H	-1.53843	-2.52431	0.57701
H	-1.4135	-4.25847	0.92721
C	-1.49816	3.72491	-2.89506
H	-1.69685	4.76922	-3.16814
H	-0.41329	3.57477	-2.91524
H	-1.94637	3.0837	-3.658
C	-4.08693	3.55274	-1.12657
H	-4.5578	2.87052	-1.83973
H	-4.48685	3.32339	-0.13447
H	-4.37473	4.57875	-1.38728
C	-1.38539	4.65573	0.00606
H	-0.31579	4.45269	0.1239
H	-1.49332	5.65972	-0.42385
H	-1.84255	4.65998	0.99835
C	-2.19669	3.38214	-1.15561
C	0.79779	-3.39286	0.16628

Mes*SnPtBu_4 E = -2407.85166467 a.u.

0 1

P	-1.64885	-0.61038	0.9395
P	2.11575	-1.34666	-0.33567
Sn	-0.11855	-2.46837	-0.20548
C	-3.01536	0.3763	0.01854
C	-3.85479	-0.10591	-1.03842
C	-3.29676	1.67679	0.57725
C	-5.05147	0.58245	-1.32081
C	-4.5211	2.28663	0.24749
C	-5.44326	1.74173	-0.65169
H	-5.70158	0.18946	-2.08645
H	-4.76395	3.2334	0.70782
C	3.0579	0.28942	-0.13733
C	3.27346	1.14743	-1.26524
C	3.69317	0.59885	1.11471
C	4.2651	2.14413	-1.16001
C	4.66285	1.61593	1.12646
C	5.00646	2.37054	-0.00048
H	4.46127	2.76455	-2.01939
H	5.17109	1.83013	2.05529
C	-2.33263	2.52	1.47328
C	-2.20026	1.96731	2.91284
C	-0.94145	2.62049	0.80291
C	-2.82278	3.98346	1.62969
H	-3.1893	1.80713	3.35917
H	-1.64777	1.02791	2.92518
H	-1.66219	2.69228	3.53653
H	-1.02905	3.09506	-0.18118
H	-0.27707	3.23577	1.42192
H	-0.4755	1.64232	0.68024

H	-2.04479	4.54841	2.15417
H	-2.99153	4.47108	0.6636
H	-3.7355	4.06038	2.23136
C	-3.52016	-1.30207	-1.97313
C	-2.12997	-1.06334	-2.61016
C	-3.60837	-2.65795	-1.23919
C	-4.49073	-1.42639	-3.17435
H	-2.18253	-0.22635	-3.31561
H	-1.37141	-0.78735	-1.87195
H	-1.79437	-1.95156	-3.15906
H	-4.64316	-2.85243	-0.93504
H	-3.29218	-3.47219	-1.90235
H	-2.98956	-2.67944	-0.34271
H	-4.12975	-2.22971	-3.82685
H	-5.50724	-1.69338	-2.86636
H	-4.5327	-0.50888	-3.77027
C	-6.7857	2.44515	-0.90466
C	-6.53306	3.86638	-1.46416
C	-7.66893	1.68369	-1.91161
C	-7.56284	2.55378	0.42979
H	-5.95206	4.47798	-0.76692
H	-5.98218	3.81944	-2.40978
H	-7.48603	4.37753	-1.64605
H	-7.88984	0.66713	-1.56787
H	-8.62255	2.20938	-2.03245
H	-7.19938	1.621	-2.89956
H	-8.5197	3.06524	0.27176
H	-7.76765	1.55988	0.84229
H	-6.99968	3.11816	1.1795
C	2.44864	1.12959	-2.58642
C	2.66459	-0.15653	-3.41407
C	0.94993	1.31117	-2.25121
C	2.8128	2.30275	-3.52925
H	2.15604	-0.06113	-4.38132
H	3.73097	-0.32207	-3.60741
H	2.25771	-1.02941	-2.90486
H	0.77983	2.28891	-1.7897
H	0.35254	1.25478	-3.16907
H	0.58821	0.54742	-1.56166
H	2.13682	2.27152	-4.39063
H	2.68441	3.27788	-3.04804
H	3.8353	2.22933	-3.91637
C	3.34703	-0.04734	2.48923
C	1.83545	0.12337	2.77048
C	3.7543	-1.53658	2.56924
C	4.0741	0.64808	3.66735
H	1.58003	1.18608	2.84441
H	1.20633	-0.3128	1.99405
H	1.57767	-0.3559	3.72319
H	4.81763	-1.66222	2.33229
H	3.5883	-1.90783	3.58789
H	3.1658	-2.14938	1.88727
H	3.71615	0.20048	4.60063
H	5.16013	0.50498	3.63511
H	3.85771	1.72051	3.71445
C	6.12134	3.42444	0.08747
C	7.44029	2.73719	0.51706
C	6.36757	4.13514	-1.2569
C	5.739	4.49629	1.13745
H	7.34004	2.24246	1.48812
H	7.74102	1.98057	-0.21573
H	8.2451	3.47737	0.59769
H	5.48371	4.68791	-1.5938
H	7.18519	4.85572	-1.14577
H	6.65279	3.42662	-2.04237
H	6.52891	5.25302	1.21162

H	4.80641	4.99838	0.85839
H	5.59993	4.05811	2.13072
C	-4.76987	-1.51042	2.27636
H	-4.93749	-0.43195	2.35818
H	-5.16623	-1.83399	1.31008
H	-5.33839	-2.01074	3.07049
C	-2.64648	-3.80579	2.24944
H	-3.2397	-4.32665	3.0126
H	-2.952	-4.1885	1.27165
H	-1.59726	-4.07776	2.41317
C	-2.31934	-1.49361	4.19891
H	-1.22746	-1.54825	4.26353
H	-2.6229	-0.4852	4.49163
H	-2.74044	-2.20289	4.92263
C	5.36441	-2.14687	-1.15069
H	5.34879	-1.29481	-1.83621
H	5.68505	-1.77821	-0.17194
H	6.10949	-2.86748	-1.5098
C	3.67945	-4.41109	0.20949
H	2.67291	-4.8195	0.34932
H	4.3213	-5.21699	-0.16856
H	4.06104	-4.1024	1.18583
C	3.14023	-3.71615	-2.71562
H	3.80466	-4.55363	-2.9637
H	2.11653	-4.10245	-2.66726
H	3.19341	-2.98765	-3.52807
C	-2.92365	-1.92326	2.44343
C	3.66002	-2.97394	-1.04026

Mes*SnPTMS_1 E = -2910.72126599 a.u.

0 1

P	1.41309	-0.78762	-1.27725
P	-2.04819	-1.98014	0.06401
Sn	0.21184	-2.97823	-0.30217
C	2.86656	0.11764	-0.40838
C	3.84478	-0.45964	0.4661
C	3.04377	1.48629	-0.83433
C	5.0293	0.25799	0.72774
C	4.26161	2.12201	-0.53154
C	5.28697	1.52539	0.20797
H	5.77733	-0.19625	1.357
H	4.41921	3.1301	-0.88504
C	-3.07876	-0.4054	0.21672
C	-3.2055	0.26911	1.47367
C	-3.86286	0.02504	-0.90779
C	-4.22075	1.23834	1.60353
C	-4.8438	1.00575	-0.68517
C	-5.07255	1.60112	0.56028
H	-4.34661	1.72433	2.55699
H	-5.45702	1.32018	-1.5166
C	1.98412	2.36809	-1.57695
C	1.75478	1.92638	-3.0453
C	0.64676	2.38182	-0.79608
C	2.42238	3.85446	-1.65888
H	2.70869	1.84554	-3.57964
H	1.23161	0.97058	-3.10019
H	1.14216	2.67681	-3.56046
H	0.80402	2.76673	0.21818
H	-0.06821	3.04101	-1.30375
H	0.19982	1.39004	-0.732
H	1.59677	4.42846	-2.09256
H	2.6369	4.28031	-0.6728
H	3.29235	4.00225	-2.30839
C	3.69459	-1.81011	1.22445
C	2.39867	-1.77851	2.06982

C	3.74986	-3.0253	0.26945
C	4.82913	-2.06103	2.25095
H	2.51121	-1.06699	2.89577
H	1.53017	-1.44558	1.49574
H	2.18933	-2.76647	2.49786
H	4.70637	-3.03768	-0.26493
H	3.66649	-3.95788	0.84018
H	2.95556	-3.01296	-0.47655
H	4.59639	-2.97909	2.80231
H	5.8029	-2.20883	1.77198
H	4.91396	-1.25012	2.98137
C	6.60506	2.27928	0.44602
C	6.31944	3.61199	1.18009
C	7.60214	1.46944	1.29657
C	7.27119	2.58112	-0.91859
H	5.65603	4.26075	0.59988
H	5.84493	3.42731	2.14989
H	7.25506	4.15725	1.3523
H	7.85958	0.51635	0.82151
H	8.52903	2.04094	1.41748
H	7.20832	1.26213	2.29782
H	8.20492	3.13654	-0.7706
H	7.50345	1.65246	-1.45096
H	6.61994	3.18189	-1.56097
C	-2.2647	0.08083	2.70239
C	-2.33266	-1.33903	3.31571
C	-0.81532	0.42484	2.28475
C	-2.60841	1.04767	3.86299
H	-1.77256	-1.3533	4.25831
H	-3.36917	-1.61812	3.53619
H	-1.89241	-2.09146	2.66072
H	-0.74489	1.47504	1.9839
H	-0.13389	0.2621	3.12815
H	-0.47375	-0.18614	1.44827
H	-1.86725	0.90589	4.65671
H	-2.56217	2.09831	3.55859
H	-3.59427	0.84681	4.2972
C	-3.6805	-0.46295	-2.37715
C	-2.23385	-0.17198	-2.84391
C	-4.02756	-1.96151	-2.55935
C	-4.60107	0.29681	-3.36497
H	-2.04381	0.90699	-2.842
H	-1.48027	-0.64008	-2.20982
H	-2.09155	-0.54183	-3.86695
H	-5.02527	-2.18006	-2.16143
H	-4.02918	-2.20643	-3.6282
H	-3.29996	-2.61329	-2.07371
H	-4.3713	-0.0468	-4.37907
H	-5.66385	0.09779	-3.18646
H	-4.43261	1.37862	-3.34158
C	-6.20035	2.63285	0.72192
C	-7.55241	1.97479	0.35375
C	-6.30676	3.17053	2.16162
C	-5.94264	3.83248	-0.22223
H	-7.55567	1.60477	-0.67624
H	-7.76588	1.1284	1.0154
H	-8.36672	2.70228	0.45197
H	-5.39493	3.69394	2.46967
H	-7.13467	3.88513	2.2244
H	-6.50529	2.36792	2.8805
H	-6.74297	4.57458	-0.11827
H	-4.99015	4.31777	0.01628
H	-5.90787	3.52266	-1.27137
Si	2.54447	-1.75931	-2.92169
Si	-3.4606	-3.5663	0.7102
C	3.99606	-0.60013	-3.48095

H	3.61564	0.38191	-3.67011
H	4.73387	-0.55393	-2.70739
H	4.43929	-0.98902	-4.37382
C	3.26863	-3.44784	-2.29873
H	3.42702	-4.09779	-3.13382
H	4.19935	-3.27451	-1.80011
H	2.57893	-3.90251	-1.61867
C	1.35741	-2.07911	-4.42243
H	0.81325	-2.98595	-4.25983
H	0.67139	-1.26317	-4.51474
H	1.93286	-2.16461	-5.32045
C	-5.19578	-2.77834	1.07335
H	-5.10684	-2.07283	1.87288
H	-5.55189	-2.28006	0.19597
H	-5.88563	-3.54752	1.35149
C	-3.63348	-4.89066	-0.69685
H	-3.06191	-5.75855	-0.44195
H	-4.66277	-5.16127	-0.80743
H	-3.27111	-4.4826	-1.61721
C	-2.78682	-4.41602	2.3188
H	-3.59331	-4.57166	3.00454
H	-2.3461	-5.35792	2.06681
H	-2.04941	-3.78714	2.77227

Mes*SnPTMS_2 E = -2910.72126599 a.u.

0 1

P	-1.8877	0.69515	-1.55667
P	1.88802	-0.57188	-1.60826
Sn	0.00023	0.00072	0.05084
C	-3.4676	0.19322	-0.62673
C	-4.1826	1.27502	-0.01143
C	-3.83698	-1.1601	-0.29808
C	-5.06127	0.97868	1.05343
C	-4.72228	-1.36103	0.77298
C	-5.30623	-0.31693	1.50265
H	-5.56248	1.79457	1.54878
H	-4.9681	-2.37289	1.0589
C	3.46603	-0.1246	-0.64488
C	3.8288	1.19899	-0.22107
C	4.19104	-1.24744	-0.10977
C	4.71908	1.33127	0.8628
C	5.07038	-1.02074	0.9648
C	5.31027	0.24375	1.50948
H	4.95203	2.32095	1.21989
H	5.5845	-1.86642	1.39802
C	-3.45443	-2.42984	-1.12041
C	-4.08257	-2.27981	-2.52982
C	-1.93846	-2.7171	-1.22466
C	-4.06016	-3.72769	-0.52689
H	-5.17533	-2.26758	-2.45291
H	-3.7777	-1.35591	-3.01762
H	-3.79294	-3.1238	-3.16803
H	-1.49267	-2.79039	-0.22445
H	-1.78471	-3.68205	-1.72256
H	-1.39303	-1.96462	-1.79196
H	-3.79025	-4.56414	-1.18056
H	-3.6671	-3.95059	0.47128
H	-5.15304	-3.69518	-0.47876
C	-4.11183	2.77706	-0.43843
C	-2.84019	3.48032	0.1007
C	-4.20383	2.9274	-1.97658
C	-5.31491	3.58275	0.12115
H	-2.74986	3.33339	1.18331
H	-1.93988	3.09877	-0.38233
H	-2.90575	4.55877	-0.09121

H	-5.11085	2.44472	-2.35776
H	-4.24521	3.99119	-2.23999
H	-3.33698	2.49755	-2.48041
H	-5.29702	4.58268	-0.32519
H	-6.27437	3.11914	-0.13189
H	-5.26423	3.7192	1.20658
C	-6.21086	-0.63028	2.7047
C	-5.40817	-1.44145	3.75088
C	-6.73964	0.64394	3.39042
C	-7.4279	-1.4651	2.23615
H	-5.0379	-2.38408	3.33581
H	-4.54457	-0.86939	4.10652
H	-6.04212	-1.67988	4.61312
H	-7.36533	1.2393	2.71618
H	-7.35482	0.36731	4.25366
H	-5.9226	1.27725	3.75324
H	-8.07852	-1.6969	3.08768
H	-8.01572	-0.9134	1.49458
H	-7.11908	-2.41267	1.78343
C	3.43165	2.52321	-0.94436
C	4.0457	2.47837	-2.36715
C	1.91303	2.80812	-1.00959
C	4.03729	3.77934	-0.2669
H	5.13928	2.48667	-2.30202
H	3.75679	1.57947	-2.90819
H	3.73004	3.35392	-2.94794
H	1.47813	2.79752	-0.00188
H	1.74815	3.80928	-1.42577
H	1.36507	2.10141	-1.63095
H	3.76119	4.65694	-0.86154
H	3.64973	3.93394	0.7462
H	5.13041	3.74738	-0.22717
C	4.12511	-2.71524	-0.64264
C	2.85518	-3.45936	-0.15626
C	4.21971	-2.75585	-2.18778
C	5.32974	-3.55605	-0.1403
H	2.76373	-3.39104	0.93406
H	1.9533	-3.04812	-0.61112
H	2.92477	-4.52099	-0.42524
H	5.12761	-2.24779	-2.53225
H	4.2617	-3.79846	-2.52488
H	3.35397	-2.29136	-2.66203
H	5.31244	-4.52314	-0.65396
H	6.28864	-3.07545	-0.36203
H	5.27927	-3.76665	0.93325
C	6.2228	0.39477	2.73733
C	7.63565	-0.14506	2.40618
C	6.36303	1.86002	3.19137
C	5.62966	-0.41833	3.91373
H	7.60929	-1.20251	2.12512
H	8.08062	0.41286	1.57517
H	8.29308	-0.04586	3.27804
H	5.39318	2.29713	3.45323
H	7.00074	1.90804	4.08086
H	6.82642	2.48342	2.4186
H	6.27579	-0.33601	4.79573
H	4.63429	-0.0469	4.18012
H	5.53519	-1.47953	3.6635
Si	-1.86791	0.09771	-3.69468
Si	1.84284	0.20038	-3.68912
C	3.65479	0.33134	-4.36976
H	3.80241	-0.40231	-5.13453
H	3.81305	1.30802	-4.77713
H	4.34829	0.16054	-3.57303
C	1.01586	1.95516	-3.70984
H	1.77092	2.7039	-3.82893

H	0.32391	2.01377	-4.52388
H	0.49665	2.11567	-2.78812
C	0.81839	-1.01053	-4.80618
H	0.32817	-1.73533	-4.19034
H	0.08665	-0.45598	-5.35567
H	1.4753	-1.50815	-5.48863
C	-1.12731	-1.6877	-3.86037
H	-0.64116	-1.95841	-2.94644
H	-1.91459	-2.38282	-4.06506
H	-0.41772	-1.7066	-4.66101
C	-0.77908	1.34577	-4.70482
H	0.14375	0.87641	-4.975
H	-1.3024	1.63982	-5.59058
H	-0.57804	2.20944	-4.10602
C	-3.68003	0.11296	-4.38718
H	-3.73541	-0.51028	-5.25517
H	-4.35066	-0.25625	-3.63962
H	-3.9535	1.11382	-4.6487

Mes*SnPTMS_3 E = -2910.72386071 a.u.

0 1

P	1.78063	0.47944	1.50718
P	-1.68028	0.02271	0.51177
Sn	0.41585	0.49376	-0.77398
C	3.54434	0.28764	0.78765
C	4.26779	1.22071	-0.03138
C	4.06455	-1.05281	0.91961
C	5.30972	0.73752	-0.84666
C	5.10853	-1.44953	0.06388
C	5.71405	-0.59838	-0.86478
H	5.81918	1.43176	-1.49532
H	5.46952	-2.46583	0.12753
C	-3.48389	-0.06864	-0.02716
C	-4.30577	1.10547	-0.05332
C	-4.0774	-1.35533	-0.27511
C	-5.70082	0.93678	-0.16805
C	-5.47644	-1.42554	-0.38148
C	-6.31503	-0.30888	-0.29513
H	-6.32743	1.81309	-0.15367
H	-5.93486	-2.3906	-0.53818
C	3.6136	-2.11258	1.9793
C	3.55082	-1.4852	3.39448
C	2.26767	-2.78905	1.61161
C	4.64128	-3.27024	2.10045
H	4.52539	-1.06552	3.66892
H	2.79826	-0.69789	3.4592
H	3.29167	-2.25859	4.1278
H	2.31322	-3.20653	0.59857
H	2.06915	-3.6135	2.30807
H	1.43392	-2.08851	1.66481
H	4.34895	-3.90003	2.94747
H	4.65821	-3.91582	1.21559
H	5.65569	-2.90406	2.2915
C	4.07618	2.76534	-0.0134
C	2.70017	3.22566	-0.54528
C	4.34383	3.26145	1.4311
C	5.1048	3.5144	-0.89908
H	2.58392	2.92564	-1.59313
H	1.86322	2.81642	0.0203
H	2.631	4.3192	-0.49941
H	5.40668	3.14054	1.66843
H	4.09118	4.32476	1.5277
H	3.78163	2.70072	2.17417
H	4.94627	4.59139	-0.77249
H	6.13801	3.30052	-0.60815

H	4.98275	3.28901	-1.96421
C	6.80739	-1.1335	-1.80247
C	6.22509	-2.2822	-2.6615
C	7.34958	-0.05109	-2.75548
C	7.99138	-1.67374	-0.96368
H	5.85188	-3.1022	-2.0401
H	5.39351	-1.92368	-3.27772
H	6.99682	-2.68779	-3.32654
H	7.8255	0.77096	-2.20941
H	8.10537	-0.49034	-3.41584
H	6.55737	0.36579	-3.3871
H	8.77909	-2.0589	-1.62199
H	8.42023	-0.88075	-0.34149
H	7.68038	-2.48796	-0.30167
C	-3.78785	2.57702	-0.04633
C	-3.00716	2.94987	1.23794
C	-2.91684	2.81037	-1.30594
C	-4.93853	3.61104	-0.13964
H	-3.5973	2.71472	2.13081
H	-2.04881	2.43392	1.29956
H	-2.80626	4.02793	1.24006
H	-3.51398	2.66623	-2.21317
H	-2.52826	3.8361	-1.30969
H	-2.06709	2.12716	-1.35025
H	-4.49627	4.61228	-0.17625
H	-5.53827	3.48807	-1.04724
H	-5.60192	3.57835	0.73186
C	-3.29443	-2.68437	-0.50785
C	-2.36124	-2.52397	-1.7337
C	-2.49723	-3.1454	0.73732
C	-4.23355	-3.86771	-0.8545
H	-2.94813	-2.30079	-2.63172
H	-1.6318	-1.72519	-1.59525
H	-1.80984	-3.45595	-1.90678
H	-3.15499	-3.21503	1.61138
H	-2.0764	-4.14084	0.55178
H	-1.66877	-2.47531	0.96931
H	-3.61365	-4.74741	-1.05746
H	-4.90383	-4.12675	-0.02723
H	-4.83231	-3.67719	-1.75143
C	-7.83971	-0.48534	-0.37699
C	-8.30954	-1.41143	0.77123
C	-8.59555	0.85118	-0.25324
C	-8.2145	-1.12587	-1.73573
H	-7.83606	-2.39658	0.71662
H	-8.0669	-0.97563	1.7464
H	-9.39497	-1.5567	0.71972
H	-8.34226	1.53895	-1.06762
H	-9.6744	0.66705	-0.30036
H	-8.38526	1.34983	0.69938
H	-9.30026	-1.26208	-1.80312
H	-7.8958	-0.48815	-2.56728
H	-7.74565	-2.10641	-1.86537
Si	-1.74672	-0.14769	2.72423
Si	1.38958	2.35436	2.62974
C	-3.57072	-0.48513	3.29234
H	-4.19123	0.33869	3.00739
H	-3.92949	-1.37947	2.82722
H	-3.59748	-0.60071	4.35574
C	-0.61028	-1.61297	3.29437
H	-0.24811	-2.13847	2.43554
H	0.21755	-1.22644	3.85132
H	-1.17348	-2.28218	3.91071
C	-1.11721	1.50611	3.51938
H	-0.21285	1.81243	3.03649
H	-1.86103	2.26573	3.39853

H	-0.93056	1.3523	4.56169
C	1.37443	1.97752	4.53273
H	0.86416	1.05375	4.70934
H	2.38041	1.9032	4.88963
H	0.87035	2.76775	5.0488
C	-0.33059	3.07834	2.10016
H	-0.88154	3.36288	2.97217
H	-0.1804	3.93558	1.47768
H	-0.87858	2.33587	1.55855
C	2.78319	3.64566	2.23731
H	2.34845	4.51433	1.78863
H	3.27841	3.92273	3.14444
H	3.49134	3.21215	1.56242

Mes*SnPTMS_4 E = -2910.72867904 a.u.

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P	-1.2355	0.53385	-0.79558
P	1.79665	-0.0794	1.656
Sn	-0.70501	-0.21493	1.6533
C	-3.10946	0.17169	-0.85722
C	-3.93116	1.34132	-0.70563
C	-3.73991	-1.12286	-0.80218
C	-5.26692	1.1729	-0.27838
C	-5.07544	-1.19614	-0.37768
C	-5.8474	-0.07298	-0.05296
H	-5.86861	2.05259	-0.11574
H	-5.53829	-2.16819	-0.29059
C	3.34466	-0.03552	0.57786
C	3.99124	-1.25214	0.18007
C	3.9566	1.22896	0.27134
C	5.28439	-1.16342	-0.37472
C	5.24479	1.21748	-0.28913
C	5.94614	0.04522	-0.59035
H	5.79075	-2.07469	-0.64712
H	5.72429	2.16193	-0.49895
C	-3.10318	-2.45283	-1.30255
C	-2.79346	-2.28627	-2.8128
C	-1.85366	-2.89172	-0.50803
C	-4.074	-3.65743	-1.20959
H	-3.73079	-2.21754	-3.37601
H	-2.22358	-1.38302	-3.02028
H	-2.23163	-3.15062	-3.18806
H	-2.10603	-3.02697	0.55091
H	-1.49314	-3.85458	-0.88977
H	-1.03214	-2.18042	-0.57427
H	-3.57489	-4.5345	-1.63648
H	-4.33727	-3.90169	-0.17444
H	-4.99352	-3.49658	-1.78099
C	-3.50136	2.8123	-1.02062
C	-2.63639	3.43107	0.10717
C	-2.76869	2.9004	-2.38273
C	-4.73414	3.74482	-1.16862
H	-3.13974	3.33169	1.07615
H	-1.65787	2.95394	0.16827
H	-2.4873	4.50061	-0.08833
H	-3.39672	2.49359	-3.18354
H	-2.5542	3.95051	-2.61532
H	-1.81878	2.36374	-2.37236
H	-4.38639	4.71776	-1.53198
H	-5.45959	3.35719	-1.89192
H	-5.24561	3.92612	-0.21727
C	-7.2797	-0.25014	0.47461
C	-7.24229	-1.08087	1.78042
C	-7.96401	1.09534	0.78317
C	-8.13538	-0.99501	-0.57904

H	-6.79626	-2.06732	1.61935
H	-6.65509	-0.56854	2.55005
H	-8.25855	-1.22941	2.16411
H	-8.06932	1.7146	-0.1145
H	-8.96961	0.91259	1.17778
H	-7.41013	1.66762	1.53541
H	-9.15883	-1.12911	-0.20923
H	-8.17989	-0.4283	-1.51537
H	-7.7286	-1.98588	-0.80488
C	3.36563	-2.68019	0.24348
C	4.29221	-3.75964	-0.37034
C	3.07475	-3.15669	1.68747
C	2.07028	-2.70959	-0.60114
H	4.53978	-3.55209	-1.41654
H	5.22128	-3.88571	0.19649
H	3.76329	-4.71829	-0.3449
H	2.25629	-2.59857	2.14298
H	2.78556	-4.21434	1.66904
H	3.96758	-3.06229	2.31569
H	1.62364	-3.71058	-0.5651
H	1.33359	-1.99665	-0.2294
H	2.29002	-2.46783	-1.64696
C	3.29152	2.62638	0.4588
C	1.97409	2.6916	-0.35002
C	3.03255	2.96927	1.94654
C	4.17576	3.77597	-0.08609
H	2.17196	2.53609	-1.4168
H	1.2463	1.94771	-0.02288
H	1.51098	3.67847	-0.23159
H	3.94586	2.8441	2.53938
H	2.71573	4.01566	2.02952
H	2.24226	2.35009	2.37266
H	3.62038	4.71374	0.01949
H	5.11097	3.88702	0.47412
H	4.40997	3.65374	-1.14901
C	7.36904	0.12857	-1.16603
C	8.28294	0.87987	-0.16756
C	7.98328	-1.2603	-1.42485
C	7.33782	0.89892	-2.50868
H	7.91733	1.89151	0.03447
H	8.33823	0.34603	0.78729
H	9.29781	0.9642	-0.57366
H	7.40822	-1.82861	-2.16425
H	8.99983	-1.14321	-1.81593
H	8.04763	-1.85331	-0.50585
H	8.34776	0.9666	-2.92971
H	6.69574	0.3888	-3.23477
H	6.95856	1.91783	-2.38264
Si	-0.03641	-0.37039	-2.43049
Si	2.58185	-0.24257	3.72608
C	-0.99334	-0.19273	-4.10868
H	-0.53425	0.57023	-4.702
H	-0.96226	-1.1226	-4.63715
H	-2.0113	0.07216	-3.91249
C	0.2607	-2.24963	-2.0513
H	1.22232	-2.54015	-2.41977
H	0.2201	-2.41097	-0.99431
H	-0.49647	-2.83427	-2.53067
C	1.67126	0.541	-2.5602
H	1.50759	1.57617	-2.77591
H	2.1962	0.44866	-1.6324
H	2.25185	0.10083	-3.34382
C	1.96685	-1.90141	4.5221
H	2.78666	-2.39057	5.00535
H	1.20331	-1.6903	5.24137
H	1.57137	-2.53827	3.75862

XL

C	4.52134	-0.22492	3.68531
H	4.87398	-1.0658	3.12542
H	4.86016	0.67871	3.2232
H	4.8996	-0.27795	4.68481
C	1.94353	1.25601	4.77983
H	1.12553	0.93867	5.39227
H	2.73547	1.61768	5.40186
H	1.61751	2.03822	4.12657

Mes*SnPHyp_1 E = -5126.50078061 a.u.

0 1

P	2.21879	-1.23025	0.26884
P	-2.23566	-1.22155	-0.28916
Sn	-0.00659	0.00672	0.00588
C	3.3461	0.29259	0.08901
C	3.69256	1.00359	1.28882
C	3.63762	0.89599	-1.18809
C	4.13967	2.33778	1.16966
C	4.07672	2.22993	-1.20576
C	4.29587	2.98982	-0.05106
H	4.36263	2.88675	2.06989
H	4.25258	2.70355	-2.15999
C	-3.35137	0.3044	-0.06414
C	-3.62397	0.88526	1.22242
C	-3.70398	1.04294	-1.25058
C	-4.04329	2.22998	1.27346
C	-4.13253	2.37468	-1.09913
C	-4.26292	3.0106	0.13837
H	-4.19468	2.68475	2.23849
H	-4.36488	2.94568	-1.98612
C	3.62062	0.16712	-2.56902
C	4.62644	-1.00387	-2.49689
C	2.23176	-0.34729	-3.01822
C	4.11327	1.07346	-3.72558
H	5.63959	-0.62766	-2.3162
H	4.37418	-1.68845	-1.68911
H	4.62831	-1.56464	-3.43937
H	1.48472	0.45472	-2.96921
H	2.29055	-0.68641	-4.06011
H	1.8823	-1.17868	-2.40904
H	4.14548	0.47247	-4.64072
H	3.43721	1.91513	-3.91245
H	5.1233	1.4599	-3.5546
C	3.64539	0.44293	2.74805
C	2.20284	0.39337	3.3135
C	4.29272	-0.95677	2.83598
C	4.45662	1.32982	3.73078
H	1.70084	1.35945	3.18473
H	1.60994	-0.37937	2.82297
H	2.23798	0.17017	4.38734
H	5.32484	-0.93224	2.46864
H	4.3063	-1.29111	3.8805
H	3.7298	-1.68708	2.25546
H	4.50969	0.81252	4.69467
H	5.48218	1.49753	3.38474
H	3.98294	2.29956	3.91688
C	4.72935	4.45967	-0.16837
C	3.65644	5.24961	-0.95654
C	4.90616	5.13333	1.20573
C	6.07964	4.54174	-0.92168
H	3.50614	4.8385	-1.95974
H	2.6932	5.22305	-0.43591
H	3.96099	6.29738	-1.06465
H	5.69187	4.651	1.79769
H	5.19412	6.18102	1.06537

H	3.97717	5.11873	1.78627
H	6.40071	5.58618	-1.01222
H	6.85763	3.9877	-0.38541
H	6.00597	4.12517	-1.93124
C	-3.60834	0.12867	2.58838
C	-4.63259	-1.02521	2.49712
C	-2.22527	-0.4166	3.01785
C	-4.08001	1.01742	3.767
H	-5.64086	-0.62962	2.33094
H	-4.39609	-1.69521	1.67237
H	-4.63795	-1.60672	3.42703
H	-1.46695	0.3757	2.9846
H	-2.28389	-0.7797	4.05163
H	-1.89074	-1.23777	2.38698
H	-4.11699	0.39707	4.66902
H	-3.38948	1.84384	3.96816
H	-5.08422	1.4242	3.61015
C	-3.67961	0.50628	-2.71907
C	-2.24387	0.45087	-3.30146
C	-4.34331	-0.8846	-2.82265
C	-4.49195	1.41929	-3.6763
H	-1.7304	1.40956	-3.16276
H	-1.65336	-0.33559	-2.83016
H	-2.2935	0.2456	-4.37831
H	-5.37129	-0.85501	-2.44424
H	-4.37132	-1.20172	-3.87223
H	-3.78247	-1.63041	-2.26002
H	-4.5613	0.92075	-4.64897
H	-5.51173	1.59124	-3.31544
H	-4.00959	2.38723	-3.8496
C	-4.66815	4.49178	0.20567
C	-6.05977	4.67876	-0.44669
C	-4.74193	5.01754	1.65188
C	-3.62664	5.34202	-0.56182
H	-6.05949	4.36824	-1.49614
H	-6.8178	4.0878	0.07868
H	-6.35768	5.73334	-0.40822
H	-3.77906	4.92363	2.16592
H	-5.01223	6.07921	1.64152
H	-5.50091	4.48906	2.2393
H	-3.90652	6.4018	-0.53276
H	-2.63252	5.23603	-0.11446
H	-3.55517	5.04228	-1.61202
Si	3.01237	-3.39645	-0.06875
Si	-3.03382	-3.38846	0.03148
Si	-1.83837	-4.64845	-1.53661
Si	-2.62079	-4.23857	2.17211
Si	-5.31313	-3.55308	-0.47175
Si	1.81329	-4.67361	1.48259
Si	2.59476	-4.21471	-2.22088
Si	5.29106	-3.57314	0.43317
C	-5.54188	-3.70798	-2.39197
H	-5.86894	-4.69773	-2.63351
H	-6.27314	-3.00014	-2.7223
H	-4.60973	-3.51152	-2.8792
C	-6.05546	-5.12109	0.39651
H	-7.04993	-5.28937	0.03929
H	-5.44767	-5.9732	0.17422
H	-6.0782	-4.96555	1.4549
C	-6.23174	-1.96662	0.16303
H	-6.34678	-2.02216	1.22537
H	-5.65945	-1.09832	-0.08885
H	-7.19563	-1.9044	-0.29734
C	-4.25595	-4.18745	3.21481
H	-4.62933	-5.18214	3.34165
H	-4.05431	-3.75722	4.17353

H	-4.98609	-3.5948	2.70435
C	-1.26343	-3.1617	3.04477
H	-0.72305	-2.60386	2.30877
H	-1.73042	-2.48717	3.73166
H	-0.58818	-3.80012	3.57519
C	-2.00055	-6.07136	2.03147
H	-1.20612	-6.23363	2.72966
H	-2.80813	-6.73886	2.24864
H	-1.64529	-6.25248	1.03855
C	-2.87229	-4.79568	-3.17152
H	-3.90781	-4.9136	-2.92926
H	-2.74165	-3.90975	-3.75715
H	-2.53768	-5.64489	-3.72989
C	-1.50281	-6.42051	-0.82191
H	-0.77448	-6.35792	-0.04055
H	-2.4125	-6.82516	-0.42996
H	-1.13637	-7.05582	-1.60101
C	-0.14892	-3.77377	-1.91646
H	0.44458	-3.74265	-1.02669
H	0.37294	-4.31981	-2.67436
H	-0.33245	-2.77644	-2.25783
C	1.97293	-6.04876	-2.10601
H	2.05723	-6.39134	-1.09584
H	0.94982	-6.09852	-2.4153
H	2.56878	-6.66798	-2.74352
C	4.22816	-4.14992	-3.26559
H	4.52979	-5.145	-3.51802
H	4.05641	-3.59111	-4.16177
H	4.99916	-3.6779	-2.69317
C	1.23696	-3.12385	-3.07528
H	0.58239	-3.7502	-3.6446
H	0.67367	-2.60525	-2.32784
H	1.70594	-2.41442	-3.72465
C	6.21164	-1.97509	-0.16881
H	6.44421	-2.06795	-1.2091
H	5.58216	-1.12296	-0.01875
H	7.1163	-1.85297	0.38939
C	5.51787	-3.76673	2.35012
H	5.79469	-4.77521	2.57648
H	6.28545	-3.10191	2.68739
H	4.59859	-3.52983	2.84377
C	6.03285	-5.12409	-0.46566
H	6.21005	-4.88927	-1.49443
H	6.95531	-5.39965	0.00129
H	5.34233	-5.93878	-0.3996
C	0.60742	-5.86786	0.54277
H	-0.22322	-5.31008	0.16353
H	1.12639	-6.33175	-0.26986
H	0.254	-6.62042	1.2163
C	0.78927	-3.49649	2.63558
H	-0.11815	-3.21563	2.14304
H	0.5572	-4.00451	3.54825
H	1.36396	-2.6201	2.85138
C	3.04906	-5.71532	2.55558
H	3.81807	-6.11418	1.92753
H	3.48847	-5.08835	3.30306
H	2.52225	-6.51797	3.02793

Mes*SnPHyp_2 E = -5126.51397700 a.u.

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P	1.62467	-1.21949	0.44957
P	-1.66634	1.19733	-0.48645
Sn	0.84127	0.98961	-0.63693
C	3.48234	-0.78676	0.33516
C	4.05673	-0.209	1.51978

C	4.23875	-0.74277	-0.89099
C	5.23085	0.56404	1.38613
C	5.39193	0.05788	-0.93207
C	5.88451	0.76369	0.17232
H	5.6365	1.03479	2.26698
H	5.93203	0.13942	-1.86409
C	-3.28126	0.3033	-0.04976
C	-4.04822	-0.35305	-1.06895
C	-3.82005	0.40462	1.28118
C	-5.37965	-0.71078	-0.77266
C	-5.15655	0.01913	1.48151
C	-5.97385	-0.4977	0.47051
H	-5.97212	-1.1691	-1.54761
H	-5.58041	0.12694	2.46912
C	3.96663	-1.61729	-2.15218
C	4.04194	-3.09622	-1.70827
C	2.62653	-1.3272	-2.86567
C	5.05375	-1.44702	-3.24255
H	5.04336	-3.32639	-1.32813
H	3.32937	-3.30827	-0.91235
H	3.83224	-3.76357	-2.55293
H	2.55942	-0.26742	-3.14133
H	2.56949	-1.91725	-3.78874
H	1.76558	-1.57934	-2.24976
H	4.83604	-2.14675	-4.05693
H	5.05918	-0.43905	-3.67204
H	6.05692	-1.68003	-2.87136
C	3.51912	-0.36672	2.97942
C	2.30847	0.55926	3.25994
C	3.14958	-1.83595	3.28604
C	4.59876	0.00936	4.02971
H	2.54246	1.59573	2.98881
H	1.42705	0.24056	2.7035
H	2.0695	0.53545	4.33095
H	4.00983	-2.49533	3.1234
H	2.84084	-1.9258	4.33457
H	2.32324	-2.17572	2.66204
H	4.22248	-0.26556	5.02091
H	5.53791	-0.53024	3.86661
H	4.80867	1.08392	4.05768
C	7.11224	1.67533	0.01946
C	6.79287	2.78286	-1.01448
C	7.50894	2.35459	1.34378
C	8.32222	0.84754	-0.47725
H	6.54375	2.36076	-1.9932
H	5.94222	3.38899	-0.68469
H	7.65838	3.4437	-1.1426
H	7.78616	1.62149	2.10932
H	8.376	3.00331	1.17774
H	6.69833	2.97692	1.7384
H	9.20023	1.49376	-0.59412
H	8.57092	0.05569	0.23748
H	8.12262	0.37723	-1.44517
C	-3.52546	-0.76749	-2.47841
C	-4.54715	-1.6312	-3.26006
C	-3.22396	0.44782	-3.38266
C	-2.26512	-1.65053	-2.33022
H	-4.83718	-2.5329	-2.71055
H	-5.45092	-1.07297	-3.5281
H	-4.07704	-1.953	-4.19563
H	-2.39363	1.03237	-2.98918
H	-2.95253	0.10126	-4.38738
H	-4.10497	1.09331	-3.47381
H	-1.88427	-1.92164	-3.32286
H	-1.46779	-1.13612	-1.79103
H	-2.50952	-2.57383	-1.79367

C	-3.03241	0.8503	2.55057
C	-1.7863	-0.0472	2.73147
C	-2.62265	2.33956	2.50826
C	-3.86006	0.67944	3.84912
H	-2.09022	-1.0863	2.89647
H	-1.12279	-0.02021	1.86592
H	-1.21207	0.28416	3.60495
H	-3.49064	2.97803	2.30474
H	-2.2065	2.6333	3.47963
H	-1.86383	2.51958	1.74813
H	-3.21614	0.93149	4.69848
H	-4.72549	1.35076	3.88848
H	-4.20263	-0.35087	3.99242
C	-7.44227	-0.84142	0.76703
C	-8.17658	0.42995	1.25787
C	-8.18555	-1.37156	-0.47383
C	-7.50929	-1.92636	1.86939
H	-7.71942	0.83806	2.16478
H	-8.15598	1.21147	0.49069
H	-9.22389	0.19807	1.4848
H	-7.74902	-2.30623	-0.843
H	-9.23041	-1.57521	-0.21501
H	-8.18117	-0.64123	-1.29042
H	-8.55368	-2.17466	2.09294
H	-6.99974	-2.84065	1.54665
H	-7.03848	-1.58908	2.79804
Si	0.79779	-3.39286	0.16628
Si	-2.19669	3.38214	-1.15561
Si	0.48579	-4.18553	-2.01315
Si	-1.29099	-3.27092	1.21401
Si	2.14994	-4.88404	1.35945
Si	-1.20022	4.9464	0.27119
Si	-1.3389	3.80306	-3.29164
Si	-4.52694	3.59245	-1.11981
C	-2.56088	4.95413	-4.26396
H	-2.84882	5.7754	-3.64146
H	-2.07756	5.32548	-5.14339
H	-3.43023	4.39638	-4.5433
C	-5.02431	5.37548	-1.70037
H	-5.3042	5.34931	-2.73279
H	-5.85006	5.72358	-1.11568
H	-4.193	6.03696	-1.57285
C	-5.31303	2.28085	-2.3137
H	-4.82684	2.32844	-3.26567
H	-5.19016	1.30217	-1.89898
H	-6.35566	2.48852	-2.43492
C	-5.17541	3.2954	0.68431
H	-5.03938	2.26721	0.94743
H	-4.62908	3.91329	1.36595
H	-6.21543	3.54184	0.7346
C	-0.69647	4.07847	1.93147
H	0.26781	4.42673	2.2377
H	-1.41645	4.31082	2.68814
H	-0.66293	3.01917	1.78429
C	-2.45853	6.37508	0.64421
H	-1.98977	7.11033	1.26435
H	-2.76684	6.82784	-0.27495
H	-3.31298	5.97505	1.14897
C	0.38046	5.68251	-0.57922
H	0.12869	6.60213	-1.06482
H	1.13179	5.86393	0.1607
H	0.75271	4.98746	-1.30258
C	0.38617	4.6767	-3.13515
H	0.94184	4.53326	-4.03823
H	0.24188	5.72361	-2.96761
H	0.92624	4.25508	-2.31328

C	-1.13083	2.12731	-4.24672
H	-1.96465	1.98424	-4.90182
H	-0.22747	2.15307	-4.81959
H	-1.0856	1.32036	-3.5455
C	-2.52484	-2.28878	0.08414
H	-3.29697	-1.85966	0.68793
H	-1.99787	-1.51048	-0.42718
H	-2.9602	-2.95451	-0.63152
C	-1.1081	-2.35956	2.91682
H	-0.60628	-1.42606	2.76965
H	-2.07804	-2.18151	3.33205
H	-0.53911	-2.96845	3.58794
C	-1.97175	-5.06333	1.5097
H	-2.03062	-5.58117	0.5752
H	-1.31397	-5.59047	2.16875
H	-2.94613	-5.00695	1.94823
C	1.83204	-4.66575	3.26074
H	1.16254	-5.42823	3.60027
H	2.75937	-4.74436	3.78874
H	1.39889	-3.70425	3.44185
C	1.7237	-6.70316	0.83721
H	1.93553	-6.83443	-0.20336
H	2.31466	-7.38657	1.41048
H	0.68584	-6.89182	1.01649
C	4.01507	-4.51951	0.96961
H	4.24075	-4.84057	-0.02582
H	4.19873	-3.46891	1.05577
H	4.63445	-5.04797	1.66387
C	0.41849	-2.68666	-3.24298
H	-0.44949	-2.77252	-3.86276
H	0.37208	-1.77247	-2.68889
H	1.29576	-2.68828	-3.85559
C	-1.17967	-5.17582	-2.10887
H	-1.57518	-5.11348	-3.10113
H	-0.99989	-6.20091	-1.86031
H	-1.88253	-4.75927	-1.41794
C	1.95988	-5.35127	-2.4945
H	1.61657	-6.36406	-2.53056
H	2.33919	-5.06887	-3.45433
H	2.73691	-5.26386	-1.7641

Mes*SnPHyp_3 E = -5126.52097202 a.u.

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P	-1.64885	-0.61038	0.9395
P	2.11575	-1.34666	-0.33567
Sn	-0.11855	-2.46837	-0.20548
C	-3.01536	0.3763	0.01854
C	-3.85479	-0.10591	-1.03842
C	-3.29676	1.67679	0.57725
C	-5.05147	0.58245	-1.32081
C	-4.5211	2.28663	0.24749
C	-5.44326	1.74173	-0.65169
H	-5.70158	0.18946	-2.08645
H	-4.76395	3.2334	0.70782
C	3.0579	0.28942	-0.13733
C	3.27346	1.14743	-1.26524
C	3.69317	0.59885	1.11471
C	4.2651	2.14413	-1.16001
C	4.66285	1.61593	1.12646
C	5.00646	2.37054	-0.00048
H	4.46127	2.76455	-2.01939
H	5.17109	1.83013	2.05529
C	-2.33263	2.52	1.47328
C	-2.20026	1.96731	2.91284
C	-0.94145	2.62049	0.80291

C	-2.82278	3.98346	1.62969
H	-3.1893	1.80713	3.35917
H	-1.64777	1.02791	2.92518
H	-1.66219	2.69228	3.53653
H	-1.02905	3.09506	-0.18118
H	-0.27707	3.23577	1.42192
H	-0.4755	1.64232	0.68024
H	-2.04479	4.54841	2.15417
H	-2.99153	4.47108	0.6636
H	-3.7355	4.06038	2.23136
C	-3.52016	-1.30207	-1.97313
C	-2.12997	-1.06334	-2.61016
C	-3.60837	-2.65795	-1.23919
C	-4.49073	-1.42639	-3.17435
H	-2.18253	-0.22635	-3.31561
H	-1.37141	-0.78735	-1.87195
H	-1.79437	-1.95156	-3.15906
H	-4.64316	-2.85243	-0.93504
H	-3.29218	-3.47219	-1.90235
H	-2.98956	-2.67944	-0.34271
H	-4.12975	-2.22971	-3.82685
H	-5.50724	-1.69338	-2.86636
H	-4.5327	-0.50888	-3.77027
C	-6.7857	2.44515	-0.90466
C	-6.53306	3.86638	-1.46416
C	-7.66893	1.68369	-1.91161
C	-7.56284	2.55378	0.42979
H	-5.95206	4.47798	-0.76692
H	-5.98218	3.81944	-2.40978
H	-7.48603	4.37753	-1.64605
H	-7.88984	0.66713	-1.56787
H	-8.62255	2.20938	-2.03245
H	-7.19938	1.621	-2.89956
H	-8.5197	3.06524	0.27176
H	-7.76765	1.55988	0.84229
H	-6.99968	3.11816	1.1795
C	2.44864	1.12959	-2.58642
C	2.66459	-0.15653	-3.41407
C	0.94993	1.31117	-2.25121
C	2.8128	2.30275	-3.52925
H	2.15604	-0.06113	-4.38132
H	3.73097	-0.32207	-3.60741
H	2.25771	-1.02941	-2.90486
H	0.77983	2.28891	-1.7897
H	0.35254	1.25478	-3.16907
H	0.58821	0.54742	-1.56166
H	2.13682	2.27152	-4.39063
H	2.68441	3.27788	-3.04804
H	3.8353	2.22933	-3.91637
C	3.34703	-0.04734	2.48923
C	1.83545	0.12337	2.77048
C	3.7543	-1.53658	2.56924
C	4.0741	0.64808	3.66735
H	1.58003	1.18608	2.84441
H	1.20633	-0.3128	1.99405
H	1.57767	-0.3559	3.72319
H	4.81763	-1.66222	2.33229
H	3.5883	-1.90783	3.58789
H	3.1658	-2.14938	1.88727
H	3.71615	0.20048	4.60063
H	5.16013	0.50498	3.63511
H	3.85771	1.72051	3.71445
C	6.12134	3.42444	0.08747
C	7.44029	2.73719	0.51706
C	6.36757	4.13514	-1.2569
C	5.739	4.49629	1.13745

H	7.34004	2.24246	1.48812
H	7.74102	1.98057	-0.21573
H	8.2451	3.47737	0.59769
H	5.48371	4.68791	-1.5938
H	7.18519	4.85572	-1.14577
H	6.65279	3.42662	-2.04237
H	6.52891	5.25302	1.21162
H	4.80641	4.99838	0.85839
H	5.59993	4.05811	2.13072
Si	-2.92365	-1.92326	2.44343
Si	3.66002	-2.97394	-1.04026
Si	5.76167	-1.95409	-1.17643
Si	3.68389	-4.7396	0.49515
Si	3.02144	-3.88577	-3.0985
Si	-2.58456	-4.22636	2.2061
Si	-2.1816	-1.39567	4.59904
Si	-5.1984	-1.41459	2.23758
C	-5.81551	-1.91564	0.46791
H	-6.01493	-2.96662	0.44403
H	-6.7109	-1.37736	0.23675
H	-5.06106	-1.67929	-0.25309
C	-6.20412	-2.39603	3.57508
H	-5.87468	-2.10797	4.5515
H	-7.24596	-2.17565	3.47072
H	-6.04641	-3.44578	3.44071
C	-5.46147	0.48962	2.49909
H	-4.72634	1.03116	1.94121
H	-6.43901	0.76428	2.16165
H	-5.36414	0.72368	3.53863
C	-2.43072	0.50086	4.9226
H	-3.41477	0.67088	5.30686
H	-1.70664	0.83946	5.63391
H	-2.30817	1.03827	4.0055
C	-3.19927	-2.41285	5.9003
H	-2.61962	-2.53272	6.79167
H	-4.10486	-1.89176	6.13113
H	-3.43464	-3.37508	5.49581
C	-0.2996	-1.83764	4.76132
H	0.21889	-1.51845	3.88144
H	0.11064	-1.34233	5.61647
H	-0.19031	-2.89589	4.87557
C	-3.61739	-5.17369	3.54754
H	-4.10027	-6.01557	3.09702
H	-2.96612	-5.51087	4.32668
H	-4.35543	-4.51712	3.95877
C	-3.15418	-4.78503	0.43777
H	-2.94505	-4.00722	-0.26662
H	-2.62617	-5.67221	0.15668
H	-4.20551	-4.9838	0.44793
C	-0.70097	-4.62978	2.43625
H	-0.1137	-3.82183	2.05255
H	-0.48908	-4.76204	3.47669
H	-0.46126	-5.52797	1.90645
C	1.68193	-2.7492	-3.92162
H	2.10652	-2.25447	-4.77008
H	0.85154	-3.34648	-4.23564
H	1.34893	-2.01977	-3.21314
C	4.57004	-4.0062	-4.2608
H	5.35849	-4.52068	-3.75231
H	4.3086	-4.54279	-5.14885
H	4.89716	-3.02157	-4.5223
C	2.28292	-5.65788	-2.8195
H	1.8471	-6.01022	-3.73099
H	3.06211	-6.32519	-2.51543
H	1.53223	-5.61563	-2.0582
C	2.76017	-6.26805	-0.2626

H	3.34261	-6.6765	-1.06186
H	2.62139	-7.01192	0.4939
H	1.80703	-5.95873	-0.63777
C	2.79194	-4.18909	2.12762
H	2.05006	-4.91392	2.39057
H	3.50973	-4.11079	2.91727
H	2.32406	-3.23891	1.97542
C	5.51935	-5.2255	0.89339
H	5.53117	-6.10215	1.50678
H	6.0424	-5.42166	-0.01921
H	5.99681	-4.42069	1.41224
C	6.25443	-1.25338	0.5642
H	7.14897	-0.6731	0.47488
H	5.46422	-0.63556	0.93671
H	6.42188	-2.06501	1.24104
C	5.69419	-0.50297	-2.46223
H	4.81686	0.08505	-2.29069
H	6.56288	0.11195	-2.35198
H	5.6656	-0.90554	-3.4532
C	7.0788	-3.26041	-1.74416
H	7.51436	-2.9484	-2.67035
H	7.84343	-3.34247	-1.00018
H	6.60506	-4.21085	-1.87507

Mes*SnPh_1 E = -2555.40672320 a.u.

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Sn	0.35083	-0.47553	-1.1939
P	-2.07409	-1.14449	-0.2903
P	1.38262	-0.04586	1.25941
C	-2.87384	-1.9346	-1.77453
C	-4.25694	-1.8272	-2.03376
C	-4.85051	-2.54126	-3.08439
H	-5.91784	-2.44336	-3.25875
C	-4.08017	-3.37946	-3.90404
C	-2.70568	-3.50535	-3.64926
H	-2.09521	-4.15844	-4.26527
C	-2.11378	-2.79893	-2.59436
C	-3.31968	0.20481	0.2327
C	-3.94131	-0.00128	1.52768
C	-5.02699	0.80877	1.89108
H	-5.50616	0.64835	2.84553
C	-5.53713	1.81694	1.06847
C	-4.88731	2.04109	-0.13642
H	-5.26731	2.84003	-0.76259
C	-3.77315	1.29163	-0.58535
C	-3.51048	-1.06119	2.59048
C	-4.28553	-0.90992	3.92571
H	-4.16626	0.08506	4.36819
H	-3.87742	-1.63575	4.63715
H	-5.35398	-1.12849	3.82054
C	-3.80329	-2.50862	2.11582
H	-4.86486	-2.61838	1.86568
H	-3.5719	-3.21136	2.92633
H	-3.21012	-2.78502	1.24393
C	-3.25465	1.85354	-1.9543
C	-4.35463	1.67815	-3.03627
H	-4.51513	0.61855	-3.25421
H	-4.0441	2.17454	-3.96337
H	-5.31053	2.11033	-2.72972
C	-2.94803	3.36968	-1.77408
H	-3.83219	3.96211	-1.53118
H	-2.52962	3.77089	-2.70473
H	-2.21494	3.51995	-0.97392
C	3.09687	0.69023	0.86307
C	4.27575	0.06241	1.37447

C	5.48112	0.24008	0.66078
H	6.35417	-0.30661	0.99279
C	5.59977	1.08843	-0.44295
C	4.49288	1.90421	-0.71886
H	4.59488	2.67886	-1.47118
C	3.25869	1.77347	-0.05968
C	4.43316	-0.71501	2.71814
C	4.90454	-2.17084	2.49058
H	4.14469	-2.75473	1.96545
H	5.09647	-2.65212	3.45701
H	5.82997	-2.21572	1.90699
C	5.52625	0.03906	3.53357
H	6.49101	0.07155	3.02148
H	5.67613	-0.46529	4.49524
H	5.21529	1.07073	3.73081
C	2.25433	2.93721	-0.31799
C	2.98872	4.2502	0.08444
H	3.25222	4.23092	1.14719
H	2.33099	5.10954	-0.09198
H	3.90749	4.40789	-0.48536
C	1.86771	3.03379	-1.81218
H	2.73902	3.2163	-2.44871
H	1.16003	3.8566	-1.96783
H	1.39771	2.10822	-2.16529
C	1.70497	-1.86399	0.80199
C	0.94022	-2.86093	1.45634
C	1.08561	-4.21384	1.13135
H	0.49209	-4.95651	1.65408
C	1.99698	-4.61305	0.13789
C	2.75105	-3.64451	-0.53575
H	3.45495	-3.93751	-1.30775
C	2.6009	-2.28347	-0.21769
H	-4.5411	-3.92924	-4.71798
H	2.11202	-5.66394	-0.10601
C	6.88457	1.21384	-1.27583
C	7.44413	2.65324	-1.16594
H	8.36676	2.74635	-1.7509
H	6.7336	3.39526	-1.5438
H	7.67018	2.90377	-0.12406
C	6.55981	0.90584	-2.75782
H	6.18993	-0.11915	-2.87003
H	5.79506	1.58275	-3.15165
H	7.45913	1.01656	-3.37516
C	7.9811	0.23655	-0.81108
H	8.30392	0.44507	0.21492
H	7.64313	-0.80431	-0.8624
H	8.85878	0.33506	-1.45925
C	0.96763	2.92751	0.53383
H	0.4942	3.91378	0.46357
H	0.22842	2.19302	0.20767
H	1.18108	2.73753	1.59053
C	3.19959	-0.74431	3.64329
H	2.75806	0.24895	3.76738
H	2.42245	-1.42593	3.29626
H	3.5191	-1.09584	4.63213
C	-1.97115	1.2692	-2.55657
H	-1.11267	1.49117	-1.90503
H	-2.04121	0.19933	-2.75397
H	-1.76941	1.77378	-3.50906
C	-6.74335	2.64779	1.4782
C	-6.47907	3.43787	2.77556
H	-6.31047	2.76262	3.62174
H	-5.59561	4.07658	2.67563
H	-7.33793	4.07273	3.02116
C	-8.009	1.7774	1.61487
H	-8.87933	2.39776	1.85723

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H	-8.21883	1.23805	0.68557
H	-7.89318	1.03621	2.41342
C	-2.02382	-0.87045	2.97038
H	-1.35888	-0.95773	2.11257
H	-1.86665	0.11827	3.41565
H	-1.73018	-1.62716	3.70919
H	0.23597	-2.56736	2.22614
H	3.22453	-1.54927	-0.71863
H	-1.05208	-2.93927	-2.40144
H	-4.87176	-1.19062	-1.40669
C	-7.00159	3.67033	0.356
H	-6.13608	4.28646	0.22879
H	-7.20837	3.15282	-0.55742
H	-7.83973	4.28216	0.61691

Mes*SnPh_2 E = -2555.41140767 a.u.

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P	1.93933	0.48083	0.44414
P	-1.9345	-0.20696	0.63164
Sn	-0.0081	-0.20187	-1.1045
C	3.6058	0.12592	-0.3738
C	4.3595	1.26134	-0.84347
C	4.19757	-1.18106	-0.42755
C	5.69241	1.06268	-1.24752
C	5.5577	-1.26565	-0.79161
C	6.33164	-0.17757	-1.19186
H	6.25915	1.91005	-1.5951
H	6.03366	-2.23712	-0.76182
C	-3.59646	-0.25658	-0.27216
C	-4.21267	0.89118	-0.86768
C	-4.33059	-1.50581	-0.2273
C	-5.57935	0.79586	-1.22426
C	-5.66266	-1.51066	-0.66303
C	-6.33033	-0.36771	-1.12028
H	-6.06748	1.68188	-1.60261
H	-6.21719	-2.43651	-0.62959
C	3.59642	-2.59985	-0.12101
C	4.24153	-3.14208	1.18155
C	2.07133	-2.75514	0.03648
C	3.94482	-3.55582	-1.30153
H	5.33371	-3.16135	1.11766
H	3.96268	-2.52279	2.03855
H	3.89607	-4.16549	1.37029
H	1.54615	-2.43804	-0.87368
H	1.85337	-3.82189	0.17109
H	1.67098	-2.23112	0.90168
H	3.51837	-4.54521	-1.10074
H	3.51575	-3.18235	-2.23791
H	5.01642	-3.69364	-1.45671
C	3.8373	2.73192	-0.93152
C	2.54399	2.83215	-1.77903
C	3.62452	3.33897	0.47937
C	4.84751	3.67278	-1.63891
H	2.68908	2.3701	-2.76212
H	1.69555	2.35821	-1.28502
H	2.284	3.8864	-1.93191
H	4.57177	3.35651	1.03053
H	3.2662	4.37162	0.38574
H	2.89116	2.77839	1.06088
H	4.39744	4.66892	-1.70465
H	5.7836	3.78147	-1.08133
H	5.07707	3.34587	-2.6591
C	7.81198	-0.37564	-1.55583
C	7.93263	-1.39569	-2.71402
C	8.48964	0.93443	-2.0004

C	8.57114	-0.9147	-0.31888
H	7.51788	-2.37128	-2.44171
H	7.39983	-1.04053	-3.60258
H	8.98599	-1.54243	-2.97992
H	8.47368	1.68964	-1.20689
H	9.5382	0.73742	-2.24897
H	8.01219	1.35823	-2.89079
H	9.62788	-1.07552	-0.56282
H	8.51457	-0.20336	0.51205
H	8.15753	-1.86759	0.0265
C	-3.63945	2.3123	-1.21028
C	-4.29625	3.35983	-0.27345
C	-2.11828	2.54685	-1.14244
C	-4.00494	2.64706	-2.6883
H	-5.38833	3.30161	-0.29756
H	-3.97026	3.21015	0.75938
H	-4.00447	4.37079	-0.58227
H	-1.58419	1.8861	-1.83793
H	-1.92074	3.57481	-1.47078
H	-1.71306	2.44513	-0.13851
H	-3.55074	3.60587	-2.9624
H	-3.61681	1.8785	-3.36574
H	-5.07881	2.73812	-2.86336
C	-3.78485	-2.88094	0.27851
C	-2.47456	-3.28159	-0.44739
C	-3.58705	-2.87909	1.81689
C	-4.7721	-4.04171	-0.01196
H	-2.5815	-3.17075	-1.53246
H	-1.62582	-2.68668	-0.10924
H	-2.23977	-4.33121	-0.23441
H	-4.53869	-2.6749	2.3208
H	-3.23356	-3.86493	2.14366
H	-2.85585	-2.13442	2.13421
H	-4.30818	-4.9764	0.31965
H	-5.71319	-3.94124	0.53887
H	-4.99385	-4.14215	-1.08026
C	-7.81208	-0.44961	-1.51971
C	-8.64353	-0.98309	-0.32819
C	-8.38927	0.91919	-1.92758
C	-7.96079	-1.41669	-2.72006
H	-8.30472	-1.97209	-0.00498
H	-8.57187	-0.30626	0.53006
H	-9.69911	-1.06748	-0.61201
H	-7.90442	1.31433	-2.82716
H	-9.45727	0.81472	-2.14758
H	-8.28622	1.65786	-1.12501
H	-9.00871	-1.46923	-3.03798
H	-7.35993	-1.07668	-3.57027
H	-7.63614	-2.43005	-2.46288
C	2.11934	-0.13096	2.18658
C	3.34485	0.07634	2.85619
C	1.04651	-0.69826	2.90085
C	3.49158	-0.28534	4.20137
H	4.18192	0.51639	2.32434
C	1.19435	-1.04981	4.25017
H	0.09355	-0.87771	2.41072
C	2.41646	-0.84846	4.90743
H	4.44279	-0.1207	4.69791
H	0.35283	-1.48219	4.78167
H	2.53013	-1.12391	5.95074
C	-2.12073	1.12335	1.91276
C	-3.34942	1.23679	2.59904
C	-1.0457	1.94046	2.31329
C	-3.49716	2.151	3.64995
H	-4.18835	0.61295	2.3084
C	-1.1947	2.8475	3.37233

H	-0.08978	1.88252	1.80028
C	-2.41982	2.96033	4.04483
H	-4.45108	2.22567	4.16272
H	-0.35142	3.46392	3.66655
H	-2.53397	3.66423	4.86264

Mes*SnPh_3 E = -2555.41400236 a.u.

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P	1.72142	-0.05796	1.53795
P	-1.68901	-0.37863	0.55962
Sn	0.40502	-0.15971	-0.79199
C	3.46661	0.0866	0.80237
C	4.07943	1.31374	0.3844
C	4.1756	-1.15221	0.60908
C	5.29023	1.24441	-0.33469
C	5.37381	-1.12439	-0.12318
C	5.93906	0.04753	-0.63688
H	5.73908	2.16288	-0.67553
H	5.89488	-2.05381	-0.29981
C	-3.51003	-0.12113	0.16773
C	-4.0941	1.18738	0.16071
C	-4.33318	-1.27538	-0.07204
C	-5.48585	1.28768	-0.04296
C	-5.70781	-1.07302	-0.27719
C	-6.31407	0.18706	-0.25818
H	-5.93734	2.26528	-0.03291
H	-6.33638	-1.93329	-0.45206
C	3.75118	-2.53533	1.19993
C	3.67102	-2.45113	2.74613
C	2.4152	-3.06387	0.6134
C	4.79424	-3.64127	0.8973
H	4.64795	-2.17773	3.16017
H	2.93514	-1.71886	3.08268
H	3.38707	-3.42848	3.15524
H	2.41524	-2.99424	-0.4815
H	2.29209	-4.1207	0.87876
H	1.54589	-2.53442	1.00707
H	4.46932	-4.56352	1.3901
H	4.87827	-3.85596	-0.17401
H	5.78637	-3.39459	1.28951
C	3.55241	2.74919	0.70011
C	2.23281	3.08077	-0.04669
C	3.43222	2.9555	2.23374
C	4.53946	3.85504	0.2389
H	2.35682	2.90589	-1.12198
H	1.37249	2.50517	0.29845
H	1.98697	4.13999	0.09428
H	4.43089	2.93429	2.6841
H	2.98491	3.93415	2.44617
H	2.8348	2.19715	2.73952
H	4.1463	4.82384	0.56599
H	5.53161	3.73689	0.68577
H	4.64415	3.89688	-0.85064
C	7.23461	-0.02015	-1.46123
C	7.00315	-0.91041	-2.70648
C	7.69913	1.36637	-1.94631
C	8.36663	-0.63232	-0.60062
H	6.70262	-1.92518	-2.42768
H	6.21703	-0.49065	-3.34344
H	7.92342	-0.98298	-3.29839
H	7.92735	2.03527	-1.10913
H	8.61234	1.25793	-2.54179
H	6.94534	1.84783	-2.57908
H	9.29626	-0.68641	-1.17955
H	8.55075	-0.02232	0.2903

H	8.11992	-1.64561	-0.26821
C	-3.32721	2.54004	0.30857
C	-2.47725	2.62485	1.60269
C	-2.44852	2.77488	-0.94536
C	-4.28754	3.75656	0.37708
H	-3.08182	2.97491	2.44669
H	-2.02893	1.66993	1.87404
H	-1.66038	3.34068	1.45377
H	-3.07551	2.85596	-1.84012
H	-1.88205	3.70785	-0.83707
H	-1.73787	1.96201	-1.10421
H	-3.68307	4.66379	0.47949
H	-4.88692	3.87334	-0.53139
H	-4.95832	3.70705	1.24194
C	-3.83327	-2.75183	-0.13481
C	-2.85082	-2.94336	-1.31683
C	-3.19636	-3.20312	1.2041
C	-4.98763	-3.75393	-0.39277
H	-3.33316	-2.66761	-2.26136
H	-1.94683	-2.34521	-1.20327
H	-2.54896	-3.99566	-1.3808
H	-3.90135	-3.05838	2.03059
H	-2.9497	-4.27027	1.1494
H	-2.27737	-2.66193	1.43353
H	-4.56297	-4.76257	-0.42842
H	-5.73464	-3.74261	0.40834
H	-5.48918	-3.57928	-1.35082
C	-7.83098	0.31243	-0.47322
C	-8.57191	-0.47449	0.63529
C	-8.31573	1.77386	-0.4287
C	-8.20556	-0.27589	-1.85535
H	-8.30153	-1.53494	0.62836
H	-8.33058	-0.07254	1.62517
H	-9.65614	-0.40288	0.48988
H	-7.85081	2.38084	-1.21348
H	-9.39941	1.80391	-0.58582
H	-8.10869	2.24163	0.54007
H	-9.28654	-0.19604	-2.02011
H	-7.69457	0.26462	-2.65939
H	-7.93211	-1.33262	-1.93424
C	1.35467	1.69252	1.87516
C	0.63355	2.44526	0.94856
C	1.79539	2.28172	3.06083
C	0.35177	3.78691	1.2075
H	0.28579	1.98112	0.01428
C	1.51405	3.62318	3.31943
H	2.364	1.68803	3.79124
C	0.79185	4.37575	2.39289
H	-0.21717	4.38009	0.47703
H	1.86127	4.08784	4.25378
H	0.57001	5.43322	2.59706
C	-1.54606	-0.10714	2.35357
C	-1.77202	-1.16096	3.23881
C	-1.2107	1.1557	2.84344
C	-1.66164	-0.95294	4.61395
H	-2.03596	-2.15633	2.85305
C	-1.10083	1.36371	4.21828
H	-1.03264	1.98646	2.14527
C	-1.32593	0.30923	5.10361
H	-1.8394	-1.78402	5.3117
H	-0.83655	2.35887	4.60466
H	-1.23906	0.47339	6.18742

Mes*SnPh_4 E = -2555.41561209 a.u.

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P	-1.08746	0.21723	-0.82885
P	1.81346	0.05822	1.72545
Sn	-0.67881	0.08169	1.80982
C	-2.97904	0.02796	-0.75763
C	-3.73405	1.24809	-0.67817
C	-3.681	-1.22802	-0.7442
C	-5.12072	1.16546	-0.43834
C	-5.06728	-1.21142	-0.51592
C	-5.80926	-0.04105	-0.3237
H	-5.68179	2.08018	-0.34293
H	-5.59654	-2.15232	-0.48275
C	3.36751	-0.00445	0.65674
C	3.97348	-1.26151	0.33642
C	3.98943	1.22104	0.23977
C	5.21555	-1.24431	-0.33029
C	5.22499	1.13658	-0.42259
C	5.8695	-0.07183	-0.70641
H	5.68771	-2.18505	-0.55978
H	5.70855	2.05231	-0.72788
C	-3.04679	-2.62753	-1.01553
C	-2.38412	-2.65848	-2.41889
C	-2.0753	-3.06479	0.11165
C	-4.10619	-3.76008	-1.06373
H	-3.15962	-2.58663	-3.18963
H	-1.67813	-1.84743	-2.59627
H	-1.85128	-3.60649	-2.56045
H	-2.59397	-3.05023	1.07736
H	-1.73415	-4.09065	-0.07183
H	-1.18506	-2.44125	0.19325
H	-3.59791	-4.69425	-1.3264
H	-4.59615	-3.91686	-0.09666
H	-4.87221	-3.58031	-1.82485
C	-3.15707	2.68498	-0.89421
C	-2.126	3.09596	0.18956
C	-2.53471	2.80252	-2.30988
C	-4.25903	3.77351	-0.83506
H	-2.50797	2.87652	1.19424
H	-1.16092	2.60557	0.05282
H	-1.94365	4.17581	0.13227
H	-3.29644	2.61051	-3.07372
H	-2.14777	3.81801	-2.45981
H	-1.71045	2.10307	-2.45854
H	-3.79518	4.74142	-1.05223
H	-5.04307	3.61459	-1.58258
H	-4.72236	3.84851	0.15516
C	-7.31746	-0.12257	-0.03862
C	-7.55202	-0.9355	1.2578
C	-7.95795	1.26628	0.14562
C	-8.02955	-0.82789	-1.21875
H	-7.15375	-1.95167	1.17548
H	-7.06604	-0.45252	2.1124
H	-8.62526	-1.01116	1.46953
H	-7.86715	1.87894	-0.75807
H	-9.02582	1.15132	0.36171
H	-7.50699	1.81292	0.98114
H	-9.10776	-0.88989	-1.02939
H	-7.87482	-0.27485	-2.15143
H	-7.65631	-1.84621	-1.36637
C	3.37031	-2.66719	0.6363
C	4.27306	-3.81998	0.12869
C	3.20151	-2.91923	2.15575
C	2.02448	-2.83658	-0.10939
H	4.43934	-3.7761	-0.9527
H	5.24329	-3.84607	0.63682
H	3.76809	-4.76813	0.34156
H	2.42341	-2.29771	2.59831

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H	2.9241	-3.967	2.32291
H	4.14206	-2.72826	2.68464
H	1.59318	-3.8187	0.11861
H	1.29978	-2.07456	0.17917
H	2.17859	-2.77188	-1.19223
C	3.40257	2.65031	0.43879
C	2.05554	2.77959	-0.3125
C	3.25299	3.01087	1.9384
C	4.31498	3.75254	-0.15614
H	2.20899	2.65942	-1.39058
H	1.32418	2.03544	0.00261
H	1.62519	3.77301	-0.13694
H	4.20608	2.87585	2.46248
H	2.95887	4.06307	2.03342
H	2.49427	2.40872	2.4386
H	3.82193	4.71927	-0.00957
H	5.28904	3.80404	0.34309
H	4.47219	3.62889	-1.23287
C	7.23367	-0.0662	-1.41489
C	8.25483	0.71377	-0.55118
C	7.78604	-1.48574	-1.64367
C	7.09594	0.62516	-2.79313
H	7.93751	1.74762	-0.38345
H	8.38008	0.23773	0.42728
H	9.231	0.7385	-1.04953
H	7.12516	-2.08154	-2.28277
H	8.7596	-1.42318	-2.14186
H	7.93143	-2.02217	-0.69945
H	8.06466	0.64233	-3.30598
H	6.38069	0.09011	-3.42697
H	6.74999	1.65891	-2.69563
C	-0.58215	-1.48679	-1.2205
C	-0.55948	-1.92055	-2.54586
C	-0.21772	-2.35958	-0.19452
C	-0.17135	-3.22658	-2.84605
H	-0.84626	-1.23287	-3.35461
C	0.16986	-3.66542	-0.49468
H	-0.23573	-2.01736	0.8504
C	0.19343	-4.09886	-1.82057
H	-0.15311	-3.56823	-3.89108
H	0.45712	-4.35352	0.31369
H	0.49919	-5.1283	-2.05698
C	2.45769	-0.01455	3.42606
C	3.05624	1.10989	3.99404
C	2.3531	-1.19571	4.16168
C	3.54934	1.05425	5.29796
H	3.13847	2.04095	3.41471
C	2.84653	-1.2514	5.46512
H	1.88118	-2.08218	3.71362
C	3.44435	-0.12624	6.03347
H	4.02081	1.94102	5.74574
H	2.76425	-2.18215	6.04513
H	3.83309	-0.17032	7.06112

Mes*SnPh_5 E = -2555.41760918 a.u.

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P	1.52787	-1.43443	-1.54916
P	-1.89938	-2.27596	0.30068
Sn	0.33612	-3.31777	-0.08303
C	2.64305	-0.11969	-0.72782
C	3.79224	-0.41576	0.07863
C	2.39351	1.24375	-1.11758
C	4.71787	0.62006	0.32335
C	3.35613	2.21568	-0.79818
C	4.54348	1.93098	-0.11805

H	5.60931	0.39285	0.88364
H	3.18103	3.23582	-1.10669
C	-2.86794	-0.66479	0.42694
C	-2.80647	0.15883	1.5966
C	-3.69863	-0.28399	-0.68296
C	-3.56382	1.34797	1.60314
C	-4.4082	0.92401	-0.5847
C	-4.35866	1.76081	0.5348
H	-3.5277	1.97459	2.47843
H	-5.03179	1.22462	-1.41322
C	1.13367	1.75119	-1.88435
C	1.16123	1.30657	-3.36978
C	-0.16457	1.29086	-1.18347
C	1.04906	3.29926	-1.91096
H	2.08211	1.65306	-3.85299
H	1.10164	0.22195	-3.47038
H	0.30966	1.74936	-3.90181
H	-0.20318	1.67296	-0.15799
H	-1.0362	1.68078	-1.72138
H	-0.26761	0.20627	-1.14827
H	0.09639	3.58076	-2.37199
H	1.07175	3.73247	-0.90483
H	1.84285	3.75515	-2.5125
C	4.08489	-1.76491	0.8118
C	2.96425	-2.00296	1.85325
C	4.25223	-2.99144	-0.1248
C	5.39968	-1.72119	1.63608
H	3.03605	-1.2689	2.66304
H	1.96858	-1.88001	1.41349
H	3.04162	-3.0071	2.2866
H	4.83325	-2.72932	-1.01516
H	4.79006	-3.78487	0.40691
H	3.3035	-3.41494	-0.45464
H	5.49552	-2.66822	2.17801
H	6.28404	-1.61618	0.99808
H	5.40294	-0.92099	2.38222
C	5.56938	3.04606	0.13953
C	4.9136	4.1661	0.9834
C	6.81293	2.54237	0.8971
C	6.03835	3.63409	-1.2136
H	4.04873	4.60335	0.47465
H	4.57354	3.77611	1.9489
H	5.6349	4.97023	1.17125
H	7.33509	1.75505	0.34214
H	7.51596	3.37078	1.03767
H	6.55679	2.15504	1.88966
H	6.75927	4.44307	-1.0463
H	6.52061	2.86405	-1.82534
H	5.20191	4.04345	-1.7885
C	-1.96257	-0.12345	2.87857
C	-2.29402	-1.5006	3.50891
C	-0.45188	-0.01275	2.56377
C	-2.23247	0.9101	4.00232
H	-1.86658	-1.55065	4.51726
H	-3.37735	-1.64109	3.59377
H	-1.88067	-2.33235	2.94009
H	-0.19473	1.01233	2.27728
H	0.13429	-0.2757	3.45276
H	-0.15396	-0.67483	1.75096
H	-1.61208	0.64576	4.865
H	-1.95831	1.92971	3.71274
H	-3.27735	0.90257	4.33172
C	-3.90488	-1.10548	-1.9941
C	-2.59463	-1.20057	-2.81377
C	-4.47805	-2.51323	-1.69038
C	-4.93624	-0.44562	-2.9451

H	-2.26836	-0.20414	-3.1297
H	-1.77847	-1.66137	-2.25801
H	-2.76823	-1.80281	-3.71377
H	-5.39375	-2.43472	-1.0934
H	-4.72585	-3.0172	-2.63227
H	-3.76784	-3.14565	-1.15638
H	-5.03367	-1.07834	-3.83338
H	-5.92966	-0.36194	-2.4908
H	-4.61627	0.5439	-3.28864
C	-5.16401	3.06992	0.55197
C	-6.67014	2.75142	0.38707
C	-4.98223	3.85817	1.86286
C	-4.70133	3.97112	-0.61885
H	-6.87405	2.23264	-0.55474
H	-7.02517	2.11546	1.20513
H	-7.25486	3.67874	0.3933
H	-3.93591	4.13907	2.02604
H	-5.56975	4.78175	1.81859
H	-5.32745	3.28773	2.73226
H	-5.27882	4.9029	-0.62985
H	-3.6405	4.22487	-0.5185
H	-4.83901	3.47959	-1.58692
C	-2.83763	-3.46286	1.31229
C	-4.09902	-3.88925	0.8972
C	-2.295	-3.94606	2.50363
C	-4.81784	-4.79971	1.67234
H	-4.52673	-3.50893	-0.04176
C	-3.01391	-4.85594	3.27877
H	-1.30045	-3.60968	2.83074
C	-4.27526	-5.28311	2.86292
H	-5.81214	-5.1361	1.34468
H	-2.58654	-5.23693	4.21774
H	-4.84174	-6.00056	3.47406
C	2.85738	-2.55241	-2.09223
C	2.82149	-3.90159	-1.74059
C	3.91304	-2.05952	-2.86025
C	3.84029	-4.75869	-2.15761
H	1.98952	-4.29036	-1.13567
C	4.93181	-2.91638	-3.27673
H	3.94115	-0.9957	-3.13733
C	4.89525	-4.26615	-2.92573
H	3.81158	-5.82246	-1.88064
H	5.76393	-2.52823	-3.88203
H	5.6984	-4.9415	-3.25434

HypSnPH_1 E = -3721.52338036 a.u.

0 1

P	-1.20835	0.25463	0.81366
P	2.15841	-1.5908	0.56386
Sn	-0.28736	-2.16699	0.37117
Si	-3.41478	0.25096	-0.00141
Si	4.19628	-2.66246	0.91281
H	-0.57609	0.97407	-0.26499
H	2.23934	-0.27031	0.01445
Si	-4.15148	2.45572	0.58086
Si	-3.52776	-0.15804	-2.35538
Si	-4.61096	-1.39978	1.25933
Si	4.15106	-3.77809	3.03119
Si	4.62507	-4.10898	-0.96007
Si	5.71882	-0.8016	0.85541
C	-2.86682	3.73388	-0.0146
H	-3.19093	4.74752	0.25264
H	-1.8958	3.55368	0.45854
H	-2.72924	3.69643	-1.09987

C	-5.84154	2.85145	-0.21798
H	-6.17427	3.85276	0.08289
H	-5.77941	2.83559	-1.31167
H	-6.61098	2.13507	0.08773
C	-4.29552	2.57942	2.47805
H	-3.35507	2.27922	2.95186
H	-4.51664	3.61117	2.77813
H	-5.09413	1.93739	2.8644
C	-5.33276	-0.5361	-2.85607
H	-5.69631	-1.45395	-2.38116
H	-6.00319	0.281	-2.56891
H	-5.40613	-0.66797	-3.94267
C	-2.92444	1.3677	-3.33004
H	-1.8981	1.63368	-3.05591
H	-2.94335	1.1612	-4.40735
H	-3.5628	2.23757	-3.14276
C	-2.42363	-1.64356	-2.82443
H	-1.36388	-1.39737	-2.68663
H	-2.65573	-2.52927	-2.22379
H	-2.56576	-1.90468	-3.88053
C	-6.46996	-0.96098	1.2632
H	-7.03524	-1.72772	1.8074
H	-6.65323	0.00118	1.75288
H	-6.86972	-0.90643	0.24516
C	-3.96478	-1.43286	3.05273
H	-4.4944	-2.19759	3.63431
H	-2.89418	-1.6605	3.08689
H	-4.11184	-0.46565	3.54291
C	-4.41423	-3.13759	0.49129
H	-4.98468	-3.87025	1.07594
H	-4.78778	-3.16591	-0.53804
H	-3.36691	-3.4581	0.48235
C	4.04546	-5.89531	-0.62473
H	4.57	-6.33497	0.23065
H	2.96995	-5.93948	-0.43099
H	4.25383	-6.51934	-1.50281
C	3.76126	-3.42195	-2.50849
H	2.67347	-3.4346	-2.382
H	4.06661	-2.39076	-2.71143
H	4.00927	-4.0343	-3.38454
C	6.51514	-4.17022	-1.23971
H	6.7414	-4.85124	-2.06966
H	6.92083	-3.18608	-1.49479
H	7.04101	-4.5373	-0.35172
C	5.78239	-0.1128	-0.92099
H	6.19256	-0.84456	-1.6243
H	4.77779	0.15863	-1.26183
H	6.41212	0.78461	-0.9605
C	7.45913	-1.36713	1.40302
H	7.82681	-2.19649	0.79109
H	8.17002	-0.53664	1.31047
H	7.45775	-1.69055	2.44972
C	5.13557	0.58951	2.02326
H	5.86112	1.41261	2.00967
H	4.16789	0.99137	1.706
H	5.03769	0.2413	3.0561
C	5.75437	-4.79527	3.24366
H	6.64178	-4.15458	3.20888
H	5.74993	-5.31424	4.2101
H	5.85329	-5.55104	2.45715
C	4.02127	-2.50423	4.44503
H	3.15373	-1.85034	4.30716
H	3.90889	-3.01741	5.40811
H	4.91606	-1.8755	4.50148
C	2.64122	-4.93764	3.10776
H	1.71687	-4.36908	2.95983

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 H                     2.6923   -5.71043   2.33471
 H                     2.58545  -5.43233   4.08521

 HypSnPH_2 E = -3721.52371298  a.u.

0 1
  P                   -1.72142   0.05796   1.53795
 P                     1.68901   0.37863   0.55962
 Sn                   -0.40502   0.15971  -0.79199
 C                    -3.44009   0.46899   0.84161
 C                    -4.34259  -0.48856   0.27176
 C                    -3.808     1.86156   0.84774
 C                    -5.49012  -0.01087  -0.39376
 C                    -4.96805   2.24506   0.15501
 C                    -5.80973   1.34217  -0.50313
 H                    -6.15589  -0.72598  -0.84828
 H                    -5.23335   3.29169   0.12801
 C                     2.10385   1.27587   2.15926
 C                     2.38977   2.67993   2.17482
 C                     2.18775   0.51323   3.37528
 C                     2.79027   3.25828   3.39696
 C                     2.58351   1.1811    4.54573
 C                     2.90054   2.54251   4.58825
 H                     3.02407   4.30929   3.41569
 H                     2.65582   0.61684   5.4634
 C                    -3.04917   2.99096   1.61645
 C                    -3.00487   2.66566   3.13187
 C                    -1.61814   3.24284   1.07155
 C                    -3.77316   4.35704   1.50546
 H                    -4.02233   2.59179   3.53172
 H                    -2.48279   1.7299    3.33873
 H                    -2.48403   3.46898   3.66722
 H                    -1.62765   3.33519  -0.02163
 H                    -1.23144   4.18382   1.48078
 H                    -0.91573   2.45893   1.35981
 H                    -3.22739   5.08513   2.11456
 H                    -3.79149   4.73919   0.47858
 H                    -4.79833   4.31574   1.88797
 C                    -4.20173  -2.04083   0.36418
 C                    -3.00482  -2.58413  -0.46118
 C                    -4.14979  -2.49124   1.84859
 C                    -5.43477  -2.78122  -0.22005
 H                    -3.07193  -2.22934  -1.49647
 H                    -2.02873  -2.30187  -0.06344
 H                    -3.03848  -3.67992  -0.47972
 H                    -5.11336  -2.28312   2.32694
 H                    -3.96865  -3.57144   1.9062
 H                    -3.38248  -1.99087   2.43909
 H                    -5.30434  -3.85491  -0.04598
 H                    -6.36728  -2.48152   0.26845
 H                    -5.53841  -2.63652  -1.30085
 C                    -7.03884   1.85505  -1.27049
 C                    -6.57843   2.82853  -2.38276
 C                    -7.8381    0.71722  -1.93384
 C                    -7.98365   2.60261  -0.2982
 H                    -6.03101   3.68236  -1.9715
 H                    -5.92064   2.32023  -3.09609
 H                    -7.4452    3.2172   -2.93063
 H                    -8.2358    0.01385  -1.19392
 H                    -8.68887   1.13891  -2.48036
 H                    -7.22736   0.1575   -2.65085
 H                    -8.86428   2.97409  -0.83559
 H                    -8.32408   1.93658   0.50196
 H                    -7.48906   3.46088   0.16749
 C                     2.25326   3.66196   0.9679
 C                     3.61399   4.21277   0.46852
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C	1.48516	2.96326	-0.18164
C	1.41616	4.91878	1.32359
H	4.23813	4.53659	1.30873
H	4.17428	3.48267	-0.11417
H	3.4388	5.0824	-0.17562
H	0.47026	2.705	0.14016
H	1.41121	3.63468	-1.0458
H	1.97996	2.04589	-0.50509
H	1.3634	5.55686	0.43533
H	0.38625	4.67519	1.60314
H	1.87303	5.50754	2.12672
C	1.86748	-1.00677	3.51953
C	0.37688	-1.28096	3.20022
C	2.80003	-1.87914	2.64129
C	2.07891	-1.51827	4.96761
H	-0.26876	-0.69449	3.86358
H	0.12415	-1.03723	2.16843
H	0.15391	-2.34323	3.35652
H	3.85024	-1.67157	2.87588
H	2.608	-2.93917	2.84648
H	2.64412	-1.71464	1.57419
H	1.83193	-2.58473	4.99278
H	3.11872	-1.41638	5.29674
H	1.42531	-1.017	5.68973
C	3.34395	3.18647	5.91175
C	4.63087	2.48815	6.41493
C	3.64076	4.69103	5.76703
C	2.22425	3.01723	6.96738
H	4.47253	1.41785	6.57952
H	5.44334	2.60001	5.68895
H	4.95467	2.93018	7.36445
H	2.75643	5.25089	5.44305
H	3.95217	5.09647	6.73585
H	4.45083	4.87895	5.05382
H	2.52943	3.46945	7.91837
H	1.30073	3.50413	6.63605
H	1.99945	1.96275	7.15507
H	-1.28749	1.33641	2.00083
H	2.86989	0.7626	-0.13652

HypSnPH_3 E = -3721.52371304 a.u.

0 1

P	-1.87401	-0.70883	-1.47576
P	1.18968	0.15504	0.75047
Sn	0.13253	-1.94306	-0.3661
Si	-3.49325	0.15797	-0.00005
Si	3.41869	0.25439	0.0055
H	-2.60788	-1.89452	-1.84957
H	0.64042	1.2252	-0.04178
Si	-5.38465	0.37536	-1.46518
Si	-3.94301	-1.35452	1.79808
Si	-2.81148	2.32837	0.76155
Si	4.28519	2.09688	1.26556
Si	4.49344	-1.79526	0.63574
Si	3.48179	0.60079	-2.36001
C	-5.65094	-1.23229	-2.45745
H	-6.52646	-1.12593	-3.11034
H	-4.78425	-1.45172	-3.08942
H	-5.8198	-2.09186	-1.80116
C	-6.96398	0.74022	-0.45237
H	-7.8138	0.89883	-1.12808
H	-7.21518	-0.09691	0.20839
H	-6.85151	1.63752	0.16439
C	-5.06453	1.80041	-2.69119
H	-4.12165	1.64247	-3.22521

H	-5.87241	1.85655	-3.43121
H	-5.00793	2.76648	-2.17874
C	-4.95983	-0.46153	3.1469
H	-4.38786	0.35461	3.60112
H	-5.88324	-0.03996	2.73627
H	-5.23397	-1.16439	3.94322
C	-4.93186	-2.85911	1.1652
H	-4.41271	-3.35419	0.33763
H	-5.06503	-3.59347	1.96915
H	-5.92502	-2.5613	0.8126
C	-2.30801	-1.98071	2.55878
H	-1.81707	-2.69594	1.88528
H	-1.61218	-1.16075	2.76373
H	-2.50152	-2.50748	3.50149
C	-4.38822	3.32466	1.18195
H	-4.1105	4.3055	1.58771
H	-5.00881	3.49274	0.29547
H	-4.99819	2.8112	1.93288
C	-1.85815	3.2306	-0.61982
H	-1.50844	4.20858	-0.26664
H	-0.98812	2.65138	-0.94463
H	-2.49453	3.3889	-1.49632
C	-1.75329	2.22111	2.34396
H	-1.44508	3.22782	2.65359
H	-2.32334	1.77864	3.16844
H	-0.84943	1.62118	2.19644
C	3.82062	-2.39472	2.31572
H	2.75102	-2.62216	2.25517
H	4.3433	-3.30598	2.63205
H	3.9546	-1.63467	3.09136
C	4.22072	-3.16489	-0.66695
H	4.7696	-4.06905	-0.3748
H	3.16148	-3.42969	-0.755
H	4.57963	-2.85943	-1.65548
C	6.37193	-1.47766	0.78012
H	6.89343	-2.41347	1.01629
H	6.78563	-1.08855	-0.15637
H	6.59668	-0.75888	1.57519
C	2.28238	-0.61281	-3.2148
H	2.45184	-1.64464	-2.88598
H	1.23915	-0.34248	-3.01261
H	2.42184	-0.58314	-4.30274
C	5.25248	0.29411	-3.00978
H	5.55426	-0.74926	-2.86834
H	5.30657	0.51611	-4.08272
H	5.98247	0.92894	-2.49684
C	2.95723	2.38286	-2.79417
H	2.91303	2.5086	-3.88304
H	1.96619	2.6143	-2.38972
H	3.66682	3.11767	-2.39897
C	5.99451	2.62938	0.59875
H	5.92114	3.00042	-0.42945
H	6.40516	3.43749	1.21685
H	6.70889	1.79984	0.61027
C	3.07754	3.56744	1.14103
H	2.09579	3.29469	1.54243
H	3.45629	4.41964	1.71902
H	2.9432	3.89238	0.10435
C	4.44221	1.58465	3.09565
H	3.47952	1.23014	3.47858
H	5.17944	0.78577	3.229
H	4.75795	2.44025	3.70542

HypSnPH_4 E = -3721.52602716 a.u.

0 1

P	1.67042	0.6074	-0.9293
P	-1.67063	0.60704	0.92986
Sn	-0.00006	-1.14938	-0.00002
Si	3.78597	0.23507	0.01823
Si	-3.78606	0.23508	-0.01814
H	1.29895	1.81177	-0.23197
H	-1.29906	1.81165	0.233
Si	5.13624	1.88801	-1.06903
Si	3.6925	0.4964	2.39477
Si	4.45711	-1.97383	-0.62656
Si	-3.69209	0.49754	-2.39454
Si	-4.4572	-1.97415	0.62553
Si	-5.13644	1.88753	1.06968
C	4.2394	3.5703	-1.02414
H	4.85266	4.33969	-1.50964
H	3.28514	3.5114	-1.558
H	4.03586	3.89473	0.00126
C	6.82927	2.05181	-0.19891
H	7.46853	2.75543	-0.74655
H	6.71455	2.43068	0.82269
H	7.35163	1.09089	-0.14806
C	5.39677	1.38958	-2.89087
H	4.43261	1.24715	-3.38997
H	5.94528	2.17509	-3.42533
H	5.96839	0.45973	-2.97855
C	5.31211	-0.14887	3.17732
H	5.44696	-1.21989	2.99101
H	6.18566	0.37618	2.77681
H	5.29555	0.00356	4.2636
C	3.46228	2.33287	2.85867
H	2.56625	2.75023	2.38721
H	3.34957	2.4359	3.94504
H	4.3225	2.9367	2.551
C	2.21928	-0.48956	3.10151
H	1.26595	-0.03106	2.81305
H	2.22535	-1.53165	2.7636
H	2.25871	-0.49385	4.19806
C	6.36255	-2.08548	-0.55713
H	6.68989	-3.10076	-0.81286
H	6.82999	-1.39392	-1.26612
H	6.73985	-1.85127	0.44387
C	3.86059	-2.33889	-2.39987
H	4.14088	-3.35843	-2.69231
H	2.77198	-2.24924	-2.47708
H	4.30107	-1.64215	-3.11952
C	3.73441	-3.29167	0.55165
H	4.07435	-4.28969	0.24758
H	4.0553	-3.12878	1.58614
H	2.63916	-3.28979	0.52961
C	-3.73442	-3.29137	-0.55331
H	-2.63917	-3.28951	-0.53119
H	-4.07437	-4.28955	-0.24977
H	-4.05524	-3.12795	-1.58774
C	-3.86078	-2.3401	2.39868
H	-4.14104	-3.35981	2.69056
H	-2.77218	-2.25045	2.47601
H	-4.30134	-1.64377	3.11867
C	-6.36263	-2.08583	0.55594
H	-6.68994	-3.10126	0.81116
H	-6.83014	-1.39463	1.26525
H	-6.73988	-1.85116	-0.44496
C	-5.39702	1.38834	2.89131
H	-5.96859	0.45843	2.97857
H	-4.43286	1.24577	3.39037
H	-5.94559	2.1736	3.42608
C	-6.82944	2.05159	0.19956

H	-7.35176	1.09067	0.14834
H	-7.46875	2.75499	0.74742
H	-6.71471	2.43083	-0.82191
C	-4.23968	3.56988	1.02553
H	-4.85299	4.33903	1.51135
H	-3.28542	3.51079	1.55936
H	-4.03615	3.89476	0.00026
C	-5.31154	-0.14731	-3.17778
H	-6.18518	0.37755	-2.77722
H	-5.29472	0.00566	-4.26398
H	-5.44645	-1.21842	-2.99205
C	-3.46175	2.33424	-2.85749
H	-2.56583	2.75137	-2.38563
H	-3.34879	2.4378	-3.94378
H	-4.32204	2.93792	-2.54971
C	-2.21875	-0.48811	-3.10147
H	-1.26546	-0.02974	-2.8127
H	-2.22487	-1.53035	-2.76399
H	-2.25802	-0.49194	-4.19803

HypSnPMe_1 E = -3800.12260562 a.u.

0 1

P	-1.20835	0.25463	0.81366
P	2.15841	-1.5908	0.56386
Sn	-0.28736	-2.16699	0.37117
Si	-3.41478	0.25096	-0.00141
Si	3.60706	0.1435	0.00107
Si	-4.15148	2.45572	0.58086
Si	-3.52776	-0.15804	-2.35538
Si	-4.61096	-1.39978	1.25933
Si	3.57842	0.45969	-2.37242
Si	2.98867	2.09199	1.26793
Si	5.70109	-0.71337	0.81656
C	-2.86682	3.73388	-0.0146
H	-3.19093	4.74752	0.25264
H	-1.8958	3.55368	0.45854
H	-2.72924	3.69643	-1.09987
C	-5.84154	2.85145	-0.21798
H	-6.17427	3.85276	0.08289
H	-5.77941	2.83559	-1.31167
H	-6.61098	2.13507	0.08773
C	-4.29552	2.57942	2.47805
H	-3.35507	2.27922	2.95186
H	-4.51664	3.61117	2.77813
H	-5.09413	1.93739	2.8644
C	-5.33276	-0.5361	-2.85607
H	-5.69631	-1.45395	-2.38116
H	-6.00319	0.281	-2.56891
H	-5.40613	-0.66797	-3.94267
C	-2.92444	1.3677	-3.33004
H	-1.8981	1.63368	-3.05591
H	-2.94335	1.1612	-4.40735
H	-3.5628	2.23757	-3.14276
C	-2.42363	-1.64356	-2.82443
H	-1.36388	-1.39737	-2.68663
H	-2.65573	-2.52927	-2.22379
H	-2.56576	-1.90468	-3.88053
C	-6.46996	-0.96098	1.2632
H	-7.03524	-1.72772	1.8074
H	-6.65323	0.00118	1.75288
H	-6.86972	-0.90643	0.24516
C	-3.96478	-1.43286	3.05273
H	-4.4944	-2.19759	3.63431
H	-2.89418	-1.6605	3.08689
H	-4.11184	-0.46565	3.54291

C	-4.41423	-3.13759	0.49129
H	-4.98468	-3.87025	1.07594
H	-4.78778	-3.16591	-0.53804
H	-3.36691	-3.4581	0.48235
C	1.82226	3.2374	0.28461
H	2.29655	3.60379	-0.63241
H	0.89287	2.72837	0.01385
H	1.56085	4.10863	0.89819
C	2.16192	1.55962	2.89546
H	1.21968	1.03757	2.69772
H	2.80725	0.88772	3.46981
H	1.94086	2.43853	3.514
C	4.57888	3.08625	1.638
H	4.32075	3.99998	2.18779
H	5.28267	2.51468	2.25134
H	5.091	3.38279	0.71625
C	5.64761	-0.75885	2.72159
H	5.55976	0.24553	3.14803
H	4.79206	-1.34922	3.06591
H	6.56216	-1.21644	3.11867
C	7.13507	0.4019	0.2264
H	6.98992	1.44311	0.5302
H	8.08278	0.05288	0.65498
H	7.23208	0.37569	-0.86451
C	6.00528	-2.48484	0.17733
H	6.98032	-2.84343	0.53063
H	5.24065	-3.175	0.54824
H	6.00358	-2.53027	-0.91608
C	4.63381	1.98854	-2.81869
H	5.67364	1.86363	-2.49878
H	4.63104	2.14861	-3.90392
H	4.24188	2.89475	-2.34461
C	4.29114	-1.07599	-3.25119
H	3.7571	-1.98395	-2.95182
H	4.19425	-0.96912	-4.33871
H	5.35267	-1.21343	-3.02012
C	1.78484	0.72581	-2.95746
H	1.16353	-0.13331	-2.68274
H	1.34649	1.62068	-2.50527
H	1.74882	0.83884	-4.04794
C	-0.41063	1.16234	-0.54727
H	-0.76696	2.17118	-0.56023
H	0.64973	1.16042	-0.40398
H	-0.64567	0.68908	-1.47768
C	3.00021	-3.06056	-0.10217
H	3.8096	-2.75363	-0.73113
H	3.38012	-3.65064	0.70554
H	2.30583	-3.6415	-0.67247

HypSnPMe_2 E = -3800.12324666 a.u.

0 1

P	-1.18941	0.15664	-0.74901
P	1.87449	-0.70711	1.47689
Sn	-0.13216	-1.94153	0.36731
Si	-3.41895	0.25429	-0.00564
Si	-4.49205	-1.79534	-0.63884
Si	-3.48372	0.59818	2.36019
Si	-4.28578	2.09783	-1.26393
C	-3.07892	3.56883	-1.13719
H	-3.45762	4.42133	-1.71478
H	-2.94565	3.89297	-0.10011
H	-2.09669	3.29693	-1.53797
C	-5.99552	2.62869	-0.5969
H	-6.4062	3.43775	-1.21374
H	-6.70968	1.79898	-0.61005

H	-5.92256	2.998	0.43196
C	-4.44193	1.58773	-3.09469
H	-4.75806	2.44385	-3.70353
H	-3.47887	1.23433	-3.47774
H	-5.17856	0.7885	-3.22928
C	-5.25456	0.28991	3.00886
H	-5.30907	0.51018	4.08213
H	-5.98456	0.92538	2.4967
H	-5.55607	-0.7533	2.86568
C	-2.96013	2.37995	2.79683
H	-3.67024	3.11504	2.40308
H	-2.91561	2.50396	3.88589
H	-1.96935	2.61255	2.39238
C	-2.28403	-0.61556	3.21439
H	-2.42414	-0.58714	4.30228
H	-2.45259	-1.64716	2.88438
H	-1.24087	-0.34423	3.01309
C	-3.81721	-2.39268	-2.31876
H	-2.74731	-2.61854	-2.25772
H	-4.33833	-3.30449	-2.63609
H	-3.95184	-1.63224	-3.09392
C	-6.37058	-1.47873	-0.7848
H	-6.89125	-2.41456	-1.02271
H	-6.78546	-1.09108	0.15179
H	-6.59498	-0.75904	-1.57914
C	-4.21993	-3.16598	0.66289
H	-4.76803	-4.07019	0.36938
H	-3.16064	-3.4303	0.75184
H	-4.58005	-2.86158	1.65131
Si	3.49355	0.15814	-0.00001
Si	2.81241	2.32861	-0.76194
Si	5.38574	0.37515	1.46413
Si	3.94156	-1.35542	-1.79763
C	5.65188	-1.23239	2.45664
H	6.52803	-1.12641	3.10874
H	4.78559	-1.45105	3.08941
H	5.81959	-2.0923	1.80049
C	5.06688	1.80059	2.69002
H	4.12409	1.64335	3.2244
H	5.87507	1.85633	3.42973
H	5.01073	2.76661	2.17742
C	4.9583	-0.46395	-3.14752
H	5.88291	-0.04392	-2.73801
H	5.23034	-1.16718	-3.94424
H	4.38711	0.35317	-3.60098
C	4.9295	-2.86048	-1.1645
H	4.41003	-3.35503	-0.3368
H	5.06213	-3.59512	-1.96831
H	5.92286	-2.56326	-0.81201
C	2.30576	-1.98065	-2.55743
H	2.49849	-2.50743	-3.50031
H	1.81481	-2.69575	-1.88379
H	1.61026	-1.16029	-2.76192
C	1.75343	2.22136	-2.3438
H	1.44575	3.22814	-2.65376
H	2.32272	1.77806	-3.16835
H	0.84924	1.62212	-2.19547
C	4.3893	3.32425	-1.18327
H	4.99874	2.81042	-1.93437
H	4.11172	4.30509	-1.58912
H	5.01037	3.49232	-0.29712
C	1.85994	3.23132	0.61972
H	1.51009	4.20923	0.2665
H	0.99006	2.65223	0.94516
H	2.49683	3.38978	1.49582
C	6.9647	0.73925	0.45046

H	6.85206	1.63623	-0.16673
H	7.8148	0.89813	1.12574
H	7.21556	-0.09827	-0.20996
C	-0.49686	1.50879	0.25322
H	0.55058	1.5997	0.05446
H	-0.98824	2.42583	0.00323
H	-0.64577	1.29579	1.29117
C	2.7992	-2.20208	1.94844
H	3.32598	-2.57908	1.09681
H	3.49804	-1.96011	2.72172
H	2.11722	-2.94597	2.30402

HypSnPMe_3 E = -3800.12714395 a.u.

0 1

P	1.86512	0.04353	-1.4569
P	-1.87509	-0.15635	-1.39057
Sn	0.06996	-1.36757	-0.21245
Si	3.79206	0.19915	-0.13277
Si	-3.81617	0.16553	-0.13024
Si	5.30605	1.38551	-1.55957
Si	3.37076	1.33845	1.92511
Si	4.54062	-2.05213	0.20845
Si	-4.78857	-2.00771	0.12784
Si	-3.33373	1.23926	1.95332
Si	-5.16499	1.54749	-1.55732
C	4.44711	2.94644	-2.24078
H	5.13138	3.49905	-2.89664
H	3.56219	2.67583	-2.82641
H	4.1307	3.61804	-1.43652
C	6.87352	1.89824	-0.59489
H	7.58347	2.39665	-1.26664
H	6.6336	2.59608	0.21494
H	7.37628	1.02987	-0.15685
C	5.7939	0.26967	-3.0269
H	4.89974	-0.09176	-3.54537
H	6.4019	0.83248	-3.74602
H	6.37645	-0.59878	-2.70093
C	4.84978	1.11115	3.11315
H	4.98787	0.0586	3.38296
H	5.78096	1.46861	2.66095
H	4.68453	1.67677	4.03847
C	3.10719	3.20271	1.61351
H	2.30907	3.37429	0.8835
H	2.82862	3.70925	2.54581
H	4.02033	3.6738	1.2343
C	1.79765	0.63193	2.74337
H	0.91135	0.86508	2.14133
H	1.85965	-0.45443	2.86738
H	1.64844	1.07737	3.73475
C	6.42087	-2.04404	0.54771
H	6.76619	-3.06393	0.75802
H	6.98114	-1.67332	-0.3173
H	6.67389	-1.41854	1.41028
C	4.19019	-3.08603	-1.35363
H	4.56783	-4.10819	-1.22617
H	3.11656	-3.14361	-1.56042
H	4.6715	-2.64818	-2.23327
C	3.66849	-2.86185	1.70268
H	4.04551	-3.8825	1.84432
H	3.85277	-2.30499	2.62777
H	2.58546	-2.9237	1.55072
C	-2.5558	-0.00084	3.17945
H	-3.25936	-0.79983	3.43723
H	-1.65276	-0.46573	2.76838

H	-2.2729	0.51224	4.10694
C	-2.10793	2.67147	1.66405
H	-1.19591	2.31313	1.17432
H	-2.54503	3.44864	1.02936
H	-1.82375	3.13088	2.61875
C	-4.94269	1.92681	2.72016
H	-4.73169	2.39989	3.68715
H	-5.4008	2.68078	2.07104
H	-5.67781	1.13233	2.88616
C	-4.53999	3.35079	-1.49562
H	-4.6687	3.78674	-0.49911
H	-3.47959	3.41379	-1.76172
H	-5.10314	3.96717	-2.20735
C	-6.9833	1.50582	-0.97276
H	-7.07596	1.79806	0.07845
H	-7.58723	2.19894	-1.57141
H	-7.41251	0.50449	-1.08676
C	-5.05374	0.91397	-3.34971
H	-5.61591	1.57278	-4.02317
H	-4.0126	0.8816	-3.68641
H	-5.46143	-0.09742	-3.44015
C	-6.29049	-1.88217	1.30165
H	-7.03053	-1.16282	0.93628
H	-6.78218	-2.8591	1.38722
H	-5.98527	-1.57235	2.3072
C	-5.35724	-2.66189	-1.56978
H	-4.54148	-2.61482	-2.29831
H	-5.68315	-3.70592	-1.48558
H	-6.19652	-2.07756	-1.96136
C	-3.53403	-3.23696	0.87266
H	-2.67592	-3.3844	0.20831
H	-3.15588	-2.89358	1.84069
H	-4.01263	-4.21309	1.02184
C	-1.33032	1.55566	-1.68149
H	-0.91106	1.95437	-0.7814
H	-0.59137	1.56821	-2.45524
H	-2.16826	2.15093	-1.97886
C	1.23243	1.74723	-1.35928
H	0.6313	1.95432	-2.2199
H	0.6397	1.85748	-0.4753
H	2.05432	2.43151	-1.32526

HypSnPMe_4 E = -3800.12735202 a.u.

0 1

P	-1.67042	-0.6074	-0.9293
P	1.67063	-0.60704	0.92986
Sn	0.00006	1.14938	-0.00002
Si	-3.78597	-0.23507	0.01823
Si	3.78606	-0.23508	-0.01814
Si	-5.13624	-1.88801	-1.06903
Si	-3.6925	-0.4964	2.39477
Si	-4.45711	1.97383	-0.62656
Si	3.69209	-0.49754	-2.39454
Si	4.4572	1.97415	0.62553
Si	5.13644	-1.88753	1.06968
C	-4.2394	-3.5703	-1.02414
H	-4.85266	-4.33969	-1.50964
H	-3.28514	-3.5114	-1.558
H	-4.03586	-3.89473	0.00126
C	-6.82927	-2.05181	-0.19891
H	-7.46853	-2.75543	-0.74655
H	-6.71455	-2.43068	0.82269
H	-7.35163	-1.09089	-0.14806
C	-5.39677	-1.38958	-2.89087

H	-4.43261	-1.24715	-3.38997
H	-5.94528	-2.17509	-3.42533
H	-5.96839	-0.45973	-2.97855
C	-5.31211	0.14887	3.17732
H	-5.44696	1.21989	2.99101
H	-6.18566	-0.37618	2.77681
H	-5.29555	-0.00356	4.2636
C	-3.46228	-2.33287	2.85867
H	-2.56625	-2.75023	2.38721
H	-3.34957	-2.4359	3.94504
H	-4.3225	-2.9367	2.551
C	-2.21928	0.48956	3.10151
H	-1.26595	0.03106	2.81305
H	-2.22535	1.53165	2.7636
H	-2.25871	0.49385	4.19806
C	-6.36255	2.08548	-0.55713
H	-6.68989	3.10076	-0.81286
H	-6.82999	1.39392	-1.26612
H	-6.73985	1.85127	0.44387
C	-3.86059	2.33889	-2.39987
H	-4.14088	3.35843	-2.69231
H	-2.77198	2.24924	-2.47708
H	-4.30107	1.64215	-3.11952
C	-3.73441	3.29167	0.55165
H	-4.07435	4.28969	0.24758
H	-4.0553	3.12878	1.58614
H	-2.63916	3.28979	0.52961
C	3.73442	3.29137	-0.55331
H	2.63917	3.28951	-0.53119
H	4.07437	4.28955	-0.24977
H	4.05524	3.12795	-1.58774
C	3.86078	2.3401	2.39868
H	4.14104	3.35981	2.69056
H	2.77218	2.25045	2.47601
H	4.30134	1.64377	3.11867
C	6.36263	2.08583	0.55594
H	6.68994	3.10126	0.81116
H	6.83014	1.39463	1.26525
H	6.73988	1.85116	-0.44496
C	5.39702	-1.38834	2.89131
H	5.96859	-0.45843	2.97857
H	4.43286	-1.24577	3.39037
H	5.94559	-2.1736	3.42608
C	6.82944	-2.05159	0.19956
H	7.35176	-1.09067	0.14834
H	7.46875	-2.75499	0.74742
H	6.71471	-2.43083	-0.82191
C	4.23968	-3.56988	1.02553
H	4.85299	-4.33903	1.51135
H	3.28542	-3.51079	1.55936
H	4.03615	-3.89476	0.00026
C	5.31154	0.14731	-3.17778
H	6.18518	-0.37755	-2.77722
H	5.29472	-0.00566	-4.26398
H	5.44645	1.21842	-2.99205
C	3.46175	-2.33424	-2.85749
H	2.56583	-2.75137	-2.38563
H	3.34879	-2.4378	-3.94378
H	4.32204	-2.93792	-2.54971
C	2.21875	0.48811	-3.10147
H	1.26546	0.02974	-2.8127
H	2.22487	1.53035	-2.76399
H	2.25802	0.49194	-4.19803
C	-1.20105	-2.12917	-0.0482
H	-0.35566	-2.57404	-0.53017
H	-0.95026	-1.89198	0.96459

H	-2.02129	-2.81615	-0.06102
C	1.20114	-2.12911	0.04936
H	0.47991	-2.66774	0.6278
H	0.77912	-1.87581	-0.90072
H	2.06836	-2.73861	-0.09667

HypSnPtBu_1 E = -4035.89245079 a.u.

0 1

P	1.19952	0.29114	0.63674
P	-2.06392	-1.49119	-0.44103
Sn	0.3374	-2.10013	-0.15047
Si	3.47479	0.24647	0.0145
Si	-3.61338	0.18671	0.03045
Si	4.11639	2.53862	0.29489
Si	4.84284	-1.22966	1.31753
Si	3.63387	-0.33048	-2.31098
Si	-4.32256	-0.15026	2.30021
Si	-2.58341	2.34668	-0.28307
Si	-5.45159	-0.01656	-1.52035
C	3.56398	3.17563	2.00795
H	3.88603	4.21586	2.14353
H	2.47223	3.1481	2.09177
H	3.98813	2.58119	2.82364
C	6.0075	2.76762	0.13717
H	6.26236	3.83341	0.19365
H	6.53887	2.25438	0.94616
H	6.38399	2.3801	-0.81482
C	3.23819	3.59106	-1.03267
H	2.1551	3.4363	-0.98334
H	3.44072	4.65716	-0.87091
H	3.57497	3.33288	-2.04217
C	6.5382	-1.4389	0.45855
H	6.4315	-1.88047	-0.53789
H	7.04917	-0.47643	0.3499
H	7.18274	-2.09907	1.05245
C	5.1566	-0.52964	3.06767
H	4.22222	-0.38227	3.61803
H	5.78352	-1.22322	3.64215
H	5.67764	0.4327	3.02123
C	4.02732	-2.94876	1.48128
H	3.05964	-2.88733	1.99086
H	3.86195	-3.40751	0.50117
H	4.67147	-3.61785	2.06556
C	5.22431	0.43358	-3.04489
H	5.3233	0.14969	-4.10011
H	5.20481	1.52711	-2.99151
H	6.11669	0.08311	-2.51568
C	2.129	0.33948	-3.27442
H	2.23847	0.11702	-4.34335
H	1.19149	-0.11288	-2.93232
H	2.03291	1.4235	-3.159
C	3.73118	-2.22262	-2.56415
H	3.79945	-2.44901	-3.63579
H	4.61391	-2.64798	-2.07447
H	2.8469	-2.73382	-2.16837
C	-1.64564	2.90751	1.27642
H	-2.29812	2.94316	2.15531
H	-0.80624	2.23484	1.47697
H	-1.23941	3.91446	1.1171
C	-1.40718	2.29928	-1.77638
H	-0.53294	1.68462	-1.54265
H	-1.89516	1.88519	-2.66409
H	-1.06048	3.31299	-2.01415
C	-3.96376	3.62759	-0.61769

H	-3.51326	4.62519	-0.69648
H	-4.48929	3.42477	-1.55633
H	-4.70091	3.65655	0.19172
C	-4.84378	0.43197	-3.27204
H	-4.50486	1.47174	-3.32506
H	-4.0078	-0.20879	-3.57167
H	-5.65298	0.3016	-4.0012
C	-6.8342	1.18886	-0.98296
H	-6.47101	2.20993	-0.84301
H	-7.61893	1.20908	-1.74983
H	-7.29459	0.85942	-0.0449
C	-6.24904	-1.7511	-1.58052
H	-7.19483	-1.6861	-2.13357
H	-5.61207	-2.47805	-2.09079
H	-6.47054	-2.13722	-0.58097
C	-5.39765	1.32556	2.86328
H	-6.28905	1.43899	2.23772
H	-5.72828	1.17493	3.89853
H	-4.83593	2.26503	2.82482
C	-5.34304	-1.75554	2.45625
H	-4.76002	-2.62475	2.13408
H	-5.63558	-1.91559	3.50147
H	-6.25652	-1.71262	1.8543
C	-2.7972	-0.2862	3.43308
H	-2.15038	-1.10732	3.10677
H	-2.20992	0.63727	3.42084
H	-3.106	-0.48253	4.46724
C	-0.26685	0.62653	3.6864
H	-0.91214	1.05786	2.9499
H	-0.77414	-0.17679	4.17857
H	0.0024	1.37197	4.40523
C	2.88756	0.87477	3.53036
H	2.60767	1.86239	3.83232
H	3.26998	0.33885	4.37383
H	3.64149	0.93347	2.77337
C	1.50158	-1.95169	3.17478
H	2.07223	-2.10186	4.06736
H	0.52814	-2.37854	3.29775
H	1.99639	-2.42321	2.35154
C	-3.54177	-3.37128	-2.85855
H	-2.90729	-4.08949	-3.33448
H	-4.56552	-3.63728	-3.02007
H	-3.35571	-2.40188	-3.27154
C	-4.84534	-3.39018	0.02877
H	-5.58341	-3.90851	-0.54698
H	-4.69822	-3.8972	0.95946
H	-5.17657	-2.3901	0.21589
C	-2.10241	-4.89121	-0.48068
H	-1.26155	-4.95784	-1.13901
H	-1.75885	-4.79205	0.5278
H	-2.69617	-5.77688	-0.56973
C	-3.17334	-3.3444	-0.95405
C	1.33471	-0.05059	2.82611

HypSnPtBu_2 E = -4035.89733293 a.u.

0 1

P	-1.89917	-0.65378	0.36079
P	1.99741	-1.03669	0.03481
Sn	0.06277	0.70214	-0.43621
Si	-3.97195	0.32013	-0.05292
Si	3.9026	0.33444	0.21069
Si	-5.43412	-1.24042	-1.15813
Si	-4.95314	1.22121	1.95997
Si	-3.63371	2.15219	-1.60064
Si	4.53647	1.80674	-1.59151

Si	3.39617	1.65782	2.16906
Si	5.7577	-1.07953	0.79799
C	-5.58748	-2.89971	-0.23135
H	-6.22912	-3.58014	-0.80523
H	-4.61482	-3.38313	-0.1029
H	-6.04067	-2.7639	0.75596
C	-7.18897	-0.49001	-1.26321
H	-7.85535	-1.17971	-1.79641
H	-7.60943	-0.32553	-0.26512
H	-7.19662	0.46532	-1.7949
C	-4.7889	-1.5922	-2.91858
H	-3.73715	-1.89637	-2.89672
H	-5.36949	-2.40072	-3.37974
H	-4.87512	-0.7091	-3.56034
C	-6.05643	2.72632	1.54034
H	-5.49786	3.53019	1.05134
H	-6.88687	2.43975	0.88608
H	-6.48425	3.13084	2.46641
C	-6.09098	-0.03384	2.84319
H	-5.56031	-0.94128	3.14081
H	-6.50965	0.42586	3.74744
H	-6.92836	-0.32434	2.19928
C	-3.55619	1.77119	3.13208
H	-2.86036	0.94793	3.3225
H	-2.9792	2.59216	2.69341
H	-3.96524	2.11238	4.09096
C	-5.34069	2.71475	-2.2547
H	-5.21503	3.63994	-2.83154
H	-5.77684	1.96447	-2.92261
H	-6.05289	2.91442	-1.44918
C	-2.59565	1.66016	-3.12684
H	-2.73828	2.40827	-3.91733
H	-1.5273	1.62612	-2.88939
H	-2.8857	0.68351	-3.5238
C	-2.80288	3.64702	-0.75182
H	-2.68226	4.4622	-1.47656
H	-3.40069	4.02433	0.08387
H	-1.81068	3.38659	-0.37008
C	2.26601	3.14223	1.74753
H	1.31491	2.8225	1.30543
H	2.03496	3.69952	2.66427
H	2.74247	3.83216	1.04363
C	2.50429	0.58407	3.466
H	2.26135	1.18703	4.35022
H	1.57612	0.16687	3.06527
H	3.12869	-0.25643	3.7834
C	4.98577	2.36005	2.96394
H	4.71436	3.01005	3.80543
H	5.62203	1.55914	3.35428
H	5.57341	2.95236	2.25608
C	5.37586	-2.00132	2.42382
H	5.34883	-1.31459	3.27651
H	4.40626	-2.50634	2.36426
H	6.14693	-2.7559	2.62328
C	7.33263	-0.01874	1.02849
H	7.19017	0.76894	1.77365
H	8.16115	-0.65587	1.36309
H	7.63687	0.45549	0.08897
C	6.14785	-2.37732	-0.54706
H	7.00624	-2.98297	-0.22972
H	5.30355	-3.05307	-0.71096
H	6.40286	-1.90769	-1.50246
C	5.40255	3.34253	-0.84864
H	6.30251	3.06062	-0.29156
H	5.70613	4.02017	-1.65671
H	4.74469	3.89827	-0.17348

C	5.80112	1.00707	-2.77842
H	5.37171	0.17672	-3.3444
H	6.15434	1.75886	-3.49546
H	6.67171	0.63199	-2.23037
C	3.01905	2.38727	-2.5904
H	2.46182	1.53777	-2.99904
H	2.33185	2.96805	-1.9664
H	3.33627	3.01966	-3.42904
C	-0.24525	-2.34284	2.84924
H	-0.38222	-1.51011	3.54642
H	-0.1034	-3.25966	3.43598
H	0.66171	-2.15923	2.26476
C	-3.30642	-2.66349	2.82672
H	-3.37826	-1.79458	3.48783
H	-4.22852	-2.74123	2.24739
H	-3.22383	-3.5591	3.45574
C	-1.58303	-4.09253	0.65004
H	-0.64143	-4.0621	0.09394
H	-1.57837	-4.99093	1.28004
H	-2.39987	-4.1832	-0.07184
C	2.40232	-4.1433	-1.3254
H	2.40485	-4.83335	-2.17844
H	3.37582	-4.20636	-0.83066
H	1.64699	-4.48332	-0.61019
C	0.30546	-2.34205	-2.72024
H	0.12281	-1.38847	-3.22888
H	0.24578	-3.13956	-3.47213
H	-0.50023	-2.49151	-1.99534
C	3.30369	-1.82451	-3.19904
H	4.31881	-1.84778	-2.79558
H	3.26541	-2.50093	-4.06248
H	3.09401	-0.81076	-3.55351
C	-1.76142	-2.53589	1.72796
C	2.02589	-2.36926	-1.90355

HypSnPtBu_3 E = -4035.89808600 a.u.

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P	-2.14887	-1.50186	-0.19389
P	1.80631	-0.89998	-0.49528
Sn	-0.04825	-0.44818	1.12492
Si	-3.65767	0.33843	-0.15944
Si	3.82535	0.16868	0.00558
Si	-5.9079	-0.38374	-0.6651
Si	-3.81271	1.90086	1.68044
Si	-2.88866	1.55993	-2.10088
Si	5.04923	1.0602	-1.88687
Si	3.31662	2.12173	1.35461
Si	5.14948	-1.30456	1.38151
C	-6.75304	-1.43285	0.69306
H	-7.79779	-1.60049	0.40009
H	-6.28758	-2.40891	0.85027
H	-6.75886	-0.90276	1.65148
C	-7.0409	1.14928	-0.84589
H	-8.01578	0.82934	-1.23621
H	-7.21312	1.62312	0.12698
H	-6.6356	1.90322	-1.52452
C	-5.92579	-1.33789	-2.31748
H	-5.1916	-2.14911	-2.32648
H	-6.91923	-1.76789	-2.49586
H	-5.6931	-0.6679	-3.15229
C	-4.58333	3.52509	1.02526
H	-3.90602	4.03001	0.32779
H	-5.53555	3.35672	0.51421
H	-4.76443	4.20667	1.86651
C	-4.92527	1.23636	3.08279

H	-4.55804	0.25765	3.39905
H	-4.90417	1.91858	3.94162
H	-5.96656	1.12896	2.76182
C	-2.13074	2.37892	2.44818
H	-1.71393	1.57444	3.06191
H	-1.39166	2.63929	1.68394
H	-2.27128	3.25743	3.09198
C	-4.20423	2.7529	-2.80638
H	-3.74206	3.36709	-3.58998
H	-5.03444	2.20387	-3.26331
H	-4.61261	3.42495	-2.04648
C	-2.40437	0.34464	-3.49075
H	-2.00016	0.90257	-4.34506
H	-1.64514	-0.36674	-3.14706
H	-3.26161	-0.24426	-3.83064
C	-1.34008	2.58425	-1.65305
H	-0.97238	3.10818	-2.54478
H	-1.55115	3.33748	-0.88633
H	-0.53163	1.94066	-1.28998
C	1.88292	3.14469	0.6288
H	0.94922	2.57538	0.62283
H	1.72795	4.04315	1.23952
H	2.08716	3.45784	-0.39901
C	2.90378	1.66125	3.16092
H	2.68865	2.57724	3.72603
H	2.0283	1.00841	3.22792
H	3.74676	1.15885	3.64696
C	4.85458	3.25825	1.42962
H	4.64121	4.09282	2.10962
H	5.73589	2.73288	1.811
H	5.1036	3.68131	0.45152
C	4.04114	-2.04257	2.74598
H	3.57936	-1.26784	3.36479
H	3.23683	-2.63852	2.30155
H	4.63215	-2.69697	3.39893
C	6.58652	-0.33831	2.19199
H	6.21649	0.45	2.85629
H	7.19601	-1.02264	2.79563
H	7.23841	0.12476	1.44502
C	5.85476	-2.76285	0.37401
H	6.46032	-3.41344	1.01633
H	5.01875	-3.35037	-0.01634
H	6.47475	-2.43361	-0.46561
C	6.79828	1.52779	-1.27266
H	7.37493	0.62911	-1.02726
H	7.33177	2.05653	-2.07285
H	6.78129	2.17331	-0.39148
C	5.33752	-0.08012	-3.3918
H	4.41661	-0.28716	-3.94415
H	6.0285	0.436	-4.0709
H	5.79109	-1.03555	-3.11367
C	4.15269	2.61334	-2.54235
H	3.1148	2.38423	-2.80615
H	4.14232	3.42427	-1.80765
H	4.66012	2.98035	-3.44311
C	3.18972	-2.71243	-2.22613
H	3.42762	-3.36363	-1.37941
H	3.18283	-3.33337	-3.13204
H	3.99702	-1.98736	-2.32851
C	1.37728	-1.40932	-3.33825
H	0.3465	-1.05376	-3.27304
H	2.03361	-0.5655	-3.57365
H	1.43166	-2.13442	-4.16306
C	0.74669	-3.15414	-1.81788
H	0.996	-3.76278	-0.94254
H	-0.25242	-2.73301	-1.67308

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 H                     0.71591  -3.81429  -2.69537
 C                    -1.50668  -3.70506   1.4786
 H                    -1.0034   -4.09532   0.58873
 H                    -0.77335  -3.13743   2.06754
 H                    -1.82186  -4.55896   2.09302
 C                    -3.81358  -3.76685   0.4018
 H                    -3.43145  -4.78571   0.27624
 H                    -4.73967  -3.82621   0.981
 H                    -4.07387  -3.3949   -0.5927
 C                    -3.29119  -2.19186   2.19177
 H                    -4.20041  -1.60319   2.0438
 H                    -3.53416  -3.03836   2.85269
 H                    -2.55689  -1.56123   2.70834
 C                    -2.73881  -2.85205   1.10565
 C                     1.80672  -2.06012  -2.04888

 HypSnPtBu_4 E = -4035.89814150  a.u.

0 1
P                     1.91131  -0.73839  -0.10463
 P                    -1.97812  -1.02897   0.03469
 Sn                   -0.02408   0.58831   0.80463
 Si                    3.9972    0.29097   0.06496
 Si                    3.81508   2.03995   1.73088
 Si                    5.55757  -1.37637   0.87445
 Si                    4.57678   1.32745  -2.03337
 C                     4.98659   0.07981  -3.41888
 H                     5.33618   0.62781  -4.30316
 H                     5.77301  -0.62158  -3.12497
 H                     4.10419  -0.49588  -3.71458
 C                     6.10926   2.44485  -1.7928
 H                     6.43155   2.84489  -2.76225
 H                     5.88663   3.29408  -1.13897
 H                     6.95085   1.8929   -1.36047
 C                     3.1084    2.3913   -2.62139
 H                     3.32193   2.82019  -3.60844
 H                     2.1992    1.78617  -2.69992
 H                     2.90174   3.21354  -1.92989
 C                     6.74626  -0.65045   2.18282
 H                     7.42157  -1.44353   2.52833
 H                     7.35949   0.15952   1.77558
 H                     6.2057   -0.26899   3.05479
 C                     6.66178  -2.07361  -0.51926
 H                     7.24593  -1.27653  -0.99224
 H                     7.36751  -2.79954  -0.09605
 H                     6.08279  -2.58071  -1.29532
 C                     4.57451  -2.7778    1.71066
 H                     5.25152  -3.5772    2.03689
 H                     4.03867  -2.39892   2.58734
 H                     3.82622  -3.2049    1.03713
 C                     2.7302    3.49436   1.13695
 H                     1.74777   3.16366   0.78881
 H                     2.57682   4.19589   1.96689
 H                     3.21838   4.04019   0.3225
 C                     5.53846   2.78161   2.10045
 H                     5.41093   3.66884   2.73415
 H                     6.18135   2.07771   2.63431
 H                     6.05952   3.09419   1.19067
 C                     3.11712   1.34206   3.36465
 H                     3.16258   2.11086   4.14631
 H                     2.07268   1.03321   3.25597
 H                     3.6905    0.47414   3.70696
 Si                   -3.82812   0.40004  -0.24038
 Si                   -3.18919   1.50059  -2.2917
 Si                   -5.7194   -0.99763  -0.77706
 Si                   -4.37784   2.02565   1.46901
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C	-6.48418	-1.85313	0.74988
H	-7.36453	-2.42847	0.43604
H	-5.78277	-2.54871	1.21978
H	-6.80587	-1.13009	1.50484
C	-5.1872	-2.35219	-2.0082
H	-4.27354	-2.85046	-1.66891
H	-5.97893	-3.10499	-2.109
H	-4.98575	-1.93326	-2.99819
C	-4.84901	3.68934	0.6535
H	-5.68353	3.57868	-0.04597
H	-5.15075	4.40235	1.43124
H	-4.00374	4.12401	0.10972
C	-5.88326	1.48645	2.51631
H	-5.68797	0.5663	3.0748
H	-6.11891	2.27619	3.2411
H	-6.77057	1.32998	1.89363
C	-2.92234	2.36665	2.65351
H	-3.25267	3.03929	3.45533
H	-2.54884	1.44766	3.11512
H	-2.08461	2.84369	2.13496
C	-1.5164	2.39919	-2.06635
H	-1.2981	3.00546	-2.9549
H	-1.51959	3.06827	-1.19878
H	-0.6933	1.68226	-1.95517
C	-4.46087	2.79532	-2.89131
H	-4.44795	3.69413	-2.26827
H	-4.21406	3.09285	-3.91845
H	-5.48103	2.40021	-2.89217
C	-2.97795	0.19638	-3.66832
H	-2.38025	0.60896	-4.49075
H	-2.47584	-0.69912	-3.28975
H	-3.94858	-0.10391	-4.07706
C	-7.08704	0.07639	-1.5729
H	-6.76334	0.48545	-2.53545
H	-7.98248	-0.53208	-1.75151
H	-7.37312	0.91369	-0.9271
C	-0.59259	-2.68923	2.73903
H	0.18071	-2.91149	1.99798
H	-0.26161	-1.81675	3.31411
H	-0.66032	-3.53849	3.43091
C	-3.45291	-1.65609	3.24674
H	-4.44494	-1.43937	2.8423
H	-3.5725	-2.37129	4.07078
H	-3.04194	-0.73079	3.66178
C	-2.97761	-4.04924	1.30636
H	-3.15405	-4.72963	2.149
H	-3.91996	-3.92416	0.76517
H	-2.26303	-4.52338	0.62637
C	0.94383	-1.57281	-3.31522
H	0.81254	-2.3266	-4.10186
H	-0.03356	-1.13315	-3.09643
H	1.59641	-0.78361	-3.7013
C	3.33637	-3.18375	-2.14319
H	4.07124	-2.4617	-2.5056
H	3.74861	-3.6907	-1.26626
H	3.1877	-3.93633	-2.92824
C	0.47683	-3.69867	-1.09325
H	0.85176	-4.14603	-0.16737
H	-0.50847	-3.26161	-0.90325
H	0.36763	-4.4958	-1.8399
C	-2.29091	-2.38706	1.92912
C	1.66352	-2.37094	-1.74766

HypSnPTMS_1 E = -4538.75852854 a.u.

0 1

Sn	-0.26119	0.52239	0.
P	-1.48619	-1.59937	0.
P	2.1888	0.52239	0.00411
Si	-0.56887	-3.13884	1.31033
Si	-1.69461	-2.04959	-2.16386
Si	2.92576	1.57079	1.81689
Si	2.93185	1.56703	-1.80835
Si	-0.50676	-2.35173	3.5131
Si	1.60874	-3.58722	0.58055
Si	-1.84168	-5.10025	1.21848
Si	2.29692	0.3682	-3.71499
Si	5.26552	1.71541	-1.72149
Si	2.0163	3.71858	-1.899
C	2.83756	-2.33044	1.40159
H	3.57168	-2.86645	1.96609
H	3.32254	-1.75645	0.63987
H	2.29622	-1.67526	2.05165
C	2.10021	-5.39506	1.0843
H	1.55336	-6.09327	0.48567
H	3.14929	-5.53615	0.92803
H	1.86904	-5.55288	2.11704
C	1.69382	-3.40789	-1.34927
H	0.70388	-3.30377	-1.74179
H	2.27053	-2.54277	-1.602
H	2.15398	-4.27822	-1.76841
C	1.1801	-1.44722	3.82928
H	1.08701	-0.80639	4.68109
H	1.94533	-2.17276	4.01071
H	1.43834	-0.86362	2.97043
C	-0.67915	-3.84563	4.73872
H	-0.49742	-3.50975	5.73825
H	-1.66789	-4.2492	4.67229
H	0.03279	-4.6019	4.4816
C	-1.96973	-1.10979	3.79752
H	-1.72084	-0.16138	3.36919
H	-2.85551	-1.48964	3.33275
H	-2.13973	-0.99337	4.8475
C	-3.4682	-4.86451	2.24924
H	-4.28612	-4.67388	1.58625
H	-3.66527	-5.75256	2.81265
H	-3.3503	-4.03707	2.91733
C	-0.81581	-6.57202	1.95679
H	-1.48122	-7.28576	2.39577
H	-0.25337	-7.04136	1.17687
H	-0.14702	-6.20068	2.70494
C	-2.29626	-5.49034	-0.62672
H	-2.67848	-6.48729	-0.69678
H	-3.0395	-4.79883	-0.9648
H	-1.42152	-5.40007	-1.2363
C	0.06528	-2.25172	-2.95475
H	0.41871	-1.29797	-3.28693
H	0.7406	-2.64816	-2.22559
H	0.00719	-2.92053	-3.78795
C	-2.69735	-3.6951	-2.38835
H	-2.71487	-4.23123	-1.46252
H	-3.69892	-3.46465	-2.68607
H	-2.2313	-4.29701	-3.14029
C	-2.6339	-0.59536	-3.0394
H	-3.67416	-0.83513	-3.11192
H	-2.51359	0.30173	-2.46874
H	-2.232	-0.45062	-4.02043
C	2.2157	-1.52343	-3.2922
H	2.54928	-1.67898	-2.2875
H	1.20747	-1.86792	-3.39063
H	2.84555	-2.0667	-3.96529
C	0.55194	0.97373	-4.30828

H	0.66895	1.64644	-5.13209
H	-0.0323	0.13165	-4.61563
H	0.05674	1.47707	-3.50434
C	3.59673	0.6604	-5.12521
H	4.5153	0.17468	-4.86986
H	3.22343	0.25741	-6.04344
H	3.76836	1.71028	-5.24013
C	5.95612	2.09027	-3.49523
H	6.9054	2.57709	-3.41285
H	6.07119	1.1732	-4.03434
H	5.27268	2.72727	-4.0168
C	5.99705	0.03534	-1.08445
H	7.03349	-0.02354	-1.34373
H	5.89177	-0.01913	-0.02103
H	5.46937	-0.77795	-1.53723
C	5.77814	3.14364	-0.51278
H	5.89279	2.7504	0.47571
H	6.7046	3.56979	-0.83678
H	5.01977	3.89847	-0.51061
C	4.85699	1.73314	1.72982
H	5.24114	1.03992	1.01095
H	5.11845	2.72934	1.43977
H	5.27654	1.5197	2.69071
C	2.43256	0.55696	3.39566
H	1.50358	0.92392	3.77938
H	2.32876	-0.47634	3.13796
H	3.19333	0.66413	4.14041
C	2.13173	3.33843	1.90933
H	1.6784	3.47607	2.86873
H	2.89079	4.07845	1.76405
H	1.38805	3.43572	1.14619
C	1.81535	4.41224	-0.09843
H	0.92172	4.01761	0.33815
H	2.65913	4.12172	0.49195
H	1.75437	5.47996	-0.13228
C	0.28023	3.64678	-2.76183
H	-0.42494	4.21526	-2.19222
H	0.35476	4.05581	-3.74776
H	-0.04666	2.62968	-2.82143
C	3.19429	4.88047	-2.91188
H	2.69186	5.80126	-3.1231
H	4.07715	5.07875	-2.3408
H	3.46358	4.40225	-3.83041

HypSnPTMS_2 E = -4538.75973535 a.u.

0 1

P	-1.69073	0.82126	-0.61635
P	2.07657	-1.04629	-0.2705
Sn	-0.38728	-1.48623	-0.60027
Si	-3.71196	0.1502	0.43479
Si	3.64117	0.63119	0.20367
Si	-4.57703	2.23937	1.26646
Si	-5.38874	-1.09732	-0.75534
Si	-3.18001	-1.15981	2.40285
Si	4.90288	1.16237	-1.78561
Si	2.45938	2.61338	0.9224
Si	5.15692	0.05999	2.0007
C	-4.64503	3.56916	-0.09648
H	-4.97889	4.5212	0.33536
H	-3.6564	3.7228	-0.53863
H	-5.34054	3.29893	-0.89742
C	-6.3435	2.03576	1.9694
H	-6.67025	2.9812	2.4209
H	-7.05654	1.78234	1.17712
H	-6.39639	1.25887	2.73764

C	-3.41852	2.87937	2.64069
H	-2.39295	2.95685	2.26738
H	-3.74039	3.87576	2.96913
H	-3.41505	2.22126	3.5155
C	-6.7324	-1.62004	0.50176
H	-6.33008	-2.306	1.25442
H	-7.16321	-0.75939	1.02212
H	-7.54428	-2.1391	-0.02348
C	-6.2519	-0.04964	-2.09922
H	-5.56561	0.25879	-2.89336
H	-7.06119	-0.63009	-2.55965
H	-6.69256	0.85441	-1.66489
C	-4.68517	-2.69592	-1.5253
H	-3.88137	-2.4961	-2.23892
H	-4.2859	-3.35629	-0.74934
H	-5.48087	-3.23663	-2.05335
C	-4.53376	-0.89997	3.72905
H	-4.32179	-1.54551	4.59092
H	-4.55705	0.13496	4.08466
H	-5.53006	-1.15484	3.35497
C	-1.51447	-0.65387	3.18155
H	-1.36925	-1.20965	4.11698
H	-0.65944	-0.87053	2.5316
H	-1.48861	0.41465	3.41033
C	-3.1198	-3.03602	2.03345
H	-2.82506	-3.5752	2.94288
H	-4.09892	-3.41567	1.72252
H	-2.3972	-3.27956	1.24709
C	1.61961	3.48312	-0.54697
H	2.28973	3.59438	-1.40589
H	0.73936	2.91155	-0.85162
H	1.28431	4.48287	-0.243
C	1.14129	2.18122	2.21997
H	0.31193	1.65597	1.74018
H	1.53756	1.55114	3.02206
H	0.74702	3.10205	2.66872
C	3.70044	3.83643	1.71029
H	3.17493	4.77391	1.93293
H	4.10333	3.45102	2.65228
H	4.53679	4.06961	1.04432
C	4.21402	0.00423	3.6581
H	3.79698	0.98426	3.91213
H	3.38687	-0.71226	3.61927
H	4.88957	-0.29592	4.46873
C	6.4935	1.4267	2.06788
H	6.06987	2.42696	2.18195
H	7.16027	1.24049	2.91946
H	7.10489	1.41776	1.15875
C	6.12342	-1.57372	1.79495
H	6.78902	-1.69318	2.65968
H	5.47645	-2.45368	1.74789
H	6.74762	-1.55774	0.89528
C	5.52135	2.96864	-1.67009
H	6.17704	3.11447	-0.80539
H	6.09493	3.21663	-2.57221
H	4.69339	3.68068	-1.59378
C	6.44772	0.05739	-1.9854
H	6.17966	-0.99109	-2.14558
H	7.02468	0.39485	-2.85571
H	7.10259	0.11366	-1.10954
C	3.80818	0.97031	-3.33094
H	3.37618	-0.03477	-3.37679
H	2.98208	1.68714	-3.32449
H	4.39962	1.13659	-4.23995
Si	2.96609	-3.20342	-0.28322
Si	-2.03816	1.03105	-2.94083

C	-0.33712	1.51151	-3.64327
H	0.00837	2.45803	-3.22076
H	0.42097	0.7512	-3.43142
H	-0.40735	1.62905	-4.73206
C	-3.26867	2.43517	-3.29387
H	-2.89558	3.38613	-2.90252
H	-3.40393	2.54034	-4.37786
H	-4.24688	2.24569	-2.84375
C	-2.61137	-0.54101	-3.85575
H	-2.54441	-0.36972	-4.93799
H	-1.98472	-1.40704	-3.61619
H	-3.64836	-0.79751	-3.62195
C	3.01353	-3.8847	1.49412
H	1.99031	-4.04921	1.84872
H	3.54722	-4.84243	1.53325
H	3.49515	-3.1917	2.18983
C	4.68036	-3.21399	-1.10217
H	5.12542	-4.21354	-1.02155
H	4.58793	-2.96818	-2.1652
H	5.36628	-2.49897	-0.64178
C	1.83438	-4.32855	-1.32393
H	0.84475	-4.45312	-0.87435
H	1.70292	-3.9336	-2.33614
H	2.29728	-5.32079	-1.40341

HypSnPTMS_3 E = -4538.76654112 a.u.

0 1

P	2.01936	-0.64958	1.62411
P	-1.32748	0.52321	0.20813
Sn	-0.0024	-1.65354	0.24015
Si	3.59432	0.1695	0.05221
Si	-3.62795	0.20054	0.02312
Si	5.77729	-0.13766	1.0304
Si	3.56912	-0.78251	-2.15621
Si	3.13036	2.52881	-0.07607
Si	-4.51022	2.32031	-0.668
Si	-3.95998	-1.42132	-1.72055
Si	-4.5733	-0.57825	2.08797
C	6.26993	-1.9681	1.278
H	7.34555	-2.021	1.49036
H	5.74008	-2.4289	2.11579
H	6.07392	-2.56811	0.38439
C	7.10161	0.61295	-0.12732
H	8.07301	0.61405	0.3836
H	7.20806	0.0165	-1.04026
H	6.87066	1.64091	-0.41825
C	5.83825	0.7508	2.71764
H	5.01119	0.43364	3.36144
H	6.78127	0.5283	3.23212
H	5.76726	1.83672	2.59466
C	4.55597	0.35281	-3.33643
H	4.05776	1.32011	-3.4635
H	5.57037	0.53963	-2.97073
H	4.6337	-0.11679	-4.32519
C	4.36172	-2.52041	-2.18435
H	3.89455	-3.18583	-1.45059
H	4.23875	-2.97171	-3.17681
H	5.43406	-2.47437	-1.96695
C	1.7949	-0.93578	-2.84982
H	1.28517	-1.81576	-2.4365
H	1.18825	-0.04934	-2.63912
H	1.83297	-1.06701	-3.93899
C	4.63498	3.48458	-0.76757
H	4.34997	4.52863	-0.94971
H	5.46728	3.48685	-0.0558

H	4.99208	3.0635	-1.71253
C	2.7526	3.20762	1.66501
H	2.44884	4.26024	1.603
H	1.95028	2.64178	2.14641
H	3.63401	3.14463	2.31149
C	1.6489	2.85952	-1.23215
H	1.40356	3.9293	-1.2239
H	1.88361	2.57971	-2.26549
H	0.75681	2.30141	-0.92736
C	-2.75789	-1.09936	-3.16557
H	-1.71396	-1.1794	-2.84597
H	-2.92574	-1.832	-3.96495
H	-2.89976	-0.09773	-3.58309
C	-3.70383	-3.2007	-1.07716
H	-3.88485	-3.91772	-1.88791
H	-2.68131	-3.35245	-0.716
H	-4.39308	-3.43769	-0.25962
C	-5.7512	-1.28276	-2.37088
H	-5.93637	-2.06943	-3.11298
H	-6.48365	-1.40017	-1.56576
H	-5.92931	-0.31753	-2.85639
C	-3.4075	-1.86767	2.87125
H	-3.22524	-2.70353	2.18743
H	-2.44038	-1.4185	3.12272
H	-3.8437	-2.27028	3.79375
C	-6.26975	-1.38837	1.74209
H	-6.17524	-2.25846	1.08396
H	-6.72302	-1.72649	2.68225
H	-6.96033	-0.68071	1.27115
C	-4.84731	0.84817	3.32891
H	-5.27978	0.45642	4.2581
H	-3.90958	1.35302	3.58157
H	-5.53744	1.5986	2.92839
C	-6.41996	2.29053	-0.6098
H	-6.78436	2.18263	0.41783
H	-6.82237	3.22962	-1.0098
H	-6.8309	1.46762	-1.20285
C	-3.89108	3.71869	0.47302
H	-2.81149	3.86187	0.363
H	-4.38472	4.66229	0.20875
H	-4.1017	3.50823	1.52609
C	-3.92813	2.69191	-2.44573
H	-2.83903	2.60322	-2.51848
H	-4.37604	2.0031	-3.16985
H	-4.2091	3.71276	-2.73273
Si	2.88726	-2.60059	2.23135
Si	-0.95748	1.76795	2.00872
C	-2.62085	2.58432	2.58347
H	-2.89101	2.2036	3.54626
H	-2.49593	3.6454	2.64173
H	-3.39304	2.35422	1.87942
C	0.33022	3.15497	1.58257
H	1.05373	3.22341	2.3679
H	0.82285	2.91417	0.66375
H	-0.1757	4.09232	1.48102
C	-0.25848	0.6523	3.43361
H	-0.64411	-0.34051	3.33106
H	0.80969	0.62774	3.37598
H	-0.55547	1.05433	4.37969
C	1.52125	-3.6762	3.09199
H	0.82595	-3.03557	3.59303
H	1.00549	-4.25474	2.3543
H	1.97891	-4.33155	3.80331
C	4.34969	-2.30027	3.47018
H	4.0339	-2.54898	4.4618
H	5.18137	-2.91512	3.19597

H	4.64042	-1.27109	3.43603
C	3.54925	-3.53021	0.66254
H	4.04266	-2.83391	0.01709
H	4.2406	-4.28953	0.96317
H	2.72961	-3.97993	0.14211

HypSnPTMS_4 E = -4538.76713165 a.u.

0 1

Sn	-0.00001	-0.51584	-0.00015
P	-2.00438	1.13466	0.00754
P	2.00435	1.1347	-0.00744
Si	-3.82877	-0.3387	0.18989
Si	-1.98141	2.49439	-1.9059
Si	1.98132	2.49386	1.9064
Si	3.82882	-0.33853	-0.19025
Si	-3.59431	-2.23169	1.66928
Si	-3.99934	-1.13153	-2.0774
Si	-5.86637	0.8449	0.67457
Si	3.99957	-1.13164	2.07695
Si	5.86644	0.84498	-0.675
Si	3.59411	-2.23153	-1.6696
C	-2.2953	-1.6862	-2.73958
H	-2.4106	-2.12827	-3.7375
H	-1.61955	-0.82816	-2.83609
H	-1.82516	-2.43517	-2.09337
C	-5.19407	-2.6197	-2.18745
H	-6.18308	-2.37433	-1.78787
H	-5.31877	-2.92102	-3.23508
H	-4.81137	-3.48408	-1.63451
C	-4.63553	0.26406	-3.21129
H	-4.06458	1.18383	-3.04807
H	-4.52913	-0.02542	-4.26422
H	-5.69328	0.48024	-3.02768
C	-2.56622	-3.63139	0.87285
H	-2.54722	-4.49995	1.54354
H	-2.99396	-3.95377	-0.08206
H	-1.53281	-3.31756	0.69416
C	-5.32594	-2.95	2.04754
H	-5.22272	-3.83325	2.69046
H	-5.96217	-2.22813	2.57005
H	-5.84007	-3.25881	1.13144
C	-2.76596	-1.74502	3.31477
H	-1.79468	-1.27062	3.14197
H	-3.38588	-1.04625	3.88571
H	-2.60348	-2.63797	3.93099
C	-6.00091	1.22471	2.5429
H	-5.15195	1.81041	2.90804
H	-6.91725	1.79185	2.74862
H	-6.04286	0.29742	3.12497
C	-7.36531	-0.24036	0.19497
H	-8.29401	0.27996	0.46186
H	-7.38892	-0.4303	-0.88331
H	-7.35812	-1.20459	0.71121
C	-5.97811	2.45185	-0.34632
H	-6.79693	3.08173	0.02326
H	-5.05276	3.03044	-0.3061
H	-6.17663	2.21905	-1.3971
C	-2.03836	1.35581	-3.42346
H	-1.31006	0.54039	-3.37187
H	-3.03179	0.90987	-3.53154
H	-1.83349	1.94984	-4.32352
C	-3.54939	3.57118	-1.94084
H	-4.44394	2.9485	-1.84289
H	-3.56751	4.32563	-1.15111
H	-3.60112	4.09028	-2.90664

C	-0.44113	3.60616	-1.99793
H	-0.33801	4.2276	-1.10419
H	0.46933	3.00664	-2.09883
H	-0.51033	4.269	-2.87004
C	4.63598	0.26369	3.21103
H	4.06543	1.1837	3.04776
H	4.52922	-0.02581	4.26392
H	5.69387	0.47946	3.02769
C	2.2955	-1.68625	2.73915
H	1.82514	-2.43488	2.09272
H	2.41086	-2.12874	3.73688
H	1.61993	-0.82812	2.83607
C	5.19419	-2.61991	2.18683
H	6.18316	-2.37464	1.78708
H	5.31903	-2.92119	3.23446
H	4.81134	-3.4843	1.634
C	7.36529	-0.24056	-0.19575
H	8.29402	0.27961	-0.46281
H	7.38909	-0.43056	0.88252
H	7.35784	-1.20477	-0.71203
C	5.97855	2.45168	0.34621
H	6.7984	3.0808	-0.02242
H	5.05382	3.03118	0.30503
H	6.1757	2.21857	1.39717
C	6.00089	1.22511	-2.54326
H	5.15201	1.81102	-2.90827
H	6.91731	1.79215	-2.74893
H	6.04267	0.29792	-3.12549
C	3.54917	3.57083	1.94166
H	4.44382	2.94833	1.84343
H	3.5671	4.32558	1.15221
H	3.60089	4.08958	2.90764
C	2.03835	1.35486	3.42364
H	1.31014	0.53937	3.3718
H	3.03183	0.90901	3.53164
H	1.83338	1.94863	4.32385
C	0.44101	3.60556	1.99874
H	0.50987	4.26772	2.8714
H	0.33835	4.22772	1.10544
H	-0.46951	3.00601	2.09878
C	2.7657	-1.7449	-3.31508
H	1.79482	-1.26967	-3.1423
H	3.38607	-1.04684	-3.88638
H	2.60244	-2.63796	-3.93092
C	2.56614	-3.63125	-0.87301
H	2.54751	-4.49997	-1.54349
H	2.99374	-3.95327	0.08208
H	1.53261	-3.31761	-0.69463
C	5.32567	-2.94992	-2.04807
H	5.22228	-3.83316	-2.69099
H	5.96187	-2.2281	-2.57067
H	5.8399	-3.25878	-1.13205

HypSnPTMS_5 E = -4538.76656008 a.u.

0 1

P	-1.32719	0.5239	0.20886
P	2.01955	-0.64924	1.62472
Sn	-0.00203	-1.65312	0.24032
Si	-3.62756	0.20049	0.02301
Si	-3.95907	-1.42069	-1.72132
Si	-4.57353	-0.57932	2.08719
Si	-4.5101	2.3204	-0.66721
C	-3.89143	3.71847	0.47445
H	-4.38531	4.66204	0.21051
H	-4.10209	3.5075	1.52742

H	-2.81188	3.86198	0.36457
C	-6.41985	2.29015	-0.60931
H	-6.82246	3.22929	-1.00901
H	-6.83053	1.46738	-1.20274
H	-6.78437	2.18179	0.41824
C	-3.92779	2.69283	-2.44469
H	-4.20987	3.71333	-2.7318
H	-2.83854	2.60546	-2.51694
H	-4.37451	2.00347	-3.16902
C	-6.26977	-1.38936	1.74005
H	-6.72355	-1.72804	2.67976
H	-6.96011	-0.68143	1.26914
H	-6.17489	-2.25906	1.08147
C	-4.84843	0.84647	3.32867
H	-5.5388	1.59674	2.92823
H	-5.28101	0.45416	4.25757
H	-3.91103	1.35171	3.5818
C	-3.4081	-1.86906	2.87046
H	-3.8446	-2.27177	3.79277
H	-3.22584	-2.70482	2.18652
H	-2.44095	-1.42014	3.12228
C	-2.75635	-1.09838	-3.16575
H	-1.71258	-1.1805	-2.84608
H	-2.92516	-1.82968	-3.96616
H	-2.89661	-0.09597	-3.58191
C	-5.74998	-1.28185	-2.37241
H	-5.93493	-2.06852	-3.11457
H	-6.48283	-1.3991	-1.56764
H	-5.92768	-0.3166	-2.85804
C	-3.70314	-3.2003	-1.07846
H	-3.88274	-3.91696	-1.88984
H	-2.68107	-3.35186	-0.71596
H	-4.39344	-3.438	-0.26201
Si	3.59423	0.1694	0.05207
Si	3.13039	2.52881	-0.07574
Si	5.77737	-0.13818	1.02978
Si	3.56804	-0.78214	-2.15656
C	6.2702	-1.96874	1.2758
H	7.34497	-2.02136	1.49248
H	5.7372	-2.43173	2.11035
H	6.07832	-2.56693	0.38006
C	5.8381	0.7489	2.71775
H	5.01141	0.43068	3.36149
H	6.7814	0.52657	3.23179
H	5.76635	1.83487	2.59568
C	4.55484	0.35343	-3.33655
H	5.56929	0.53998	-2.97088
H	4.63243	-0.11582	-4.32549
H	4.05676	1.32085	-3.46325
C	4.3604	-2.52013	-2.18525
H	3.89398	-3.18537	-1.45085
H	4.23641	-2.97163	-3.17748
H	5.43297	-2.4741	-1.96896
C	1.79362	-0.93491	-2.84977
H	1.83137	-1.06545	-3.93903
H	1.284	-1.81515	-2.43686
H	1.18711	-0.04855	-2.63834
C	1.6491	2.85982	-1.23195
H	1.40449	3.92977	-1.2243
H	1.88348	2.57922	-2.26515
H	0.75668	2.30251	-0.92666
C	4.63509	3.48496	-0.76651
H	4.99244	3.06439	-1.7116
H	4.35001	4.52907	-0.94817
H	5.46723	3.48697	-0.05455
C	2.75222	3.2071	1.66546

H	2.44938	4.26	1.6038
H	1.94914	2.64169	2.14611
H	3.63318	3.14306	2.31246
C	7.10171	0.6135	-0.12721
H	6.8708	1.64173	-0.4172
H	8.07311	0.61409	0.38371
H	7.20817	0.0179	-1.04072
Si	-0.9589	1.7658	2.01176
Si	2.88725	-2.60024	2.23225
C	1.52086	-3.676	3.09209
H	0.81261	-3.03466	3.57373
H	1.02071	-4.27142	2.35709
H	1.97563	-4.31527	3.81971
C	3.5501	-3.5297	0.66371
H	4.00636	-2.8265	-0.0013
H	4.27309	-4.26031	0.96105
H	2.73647	-4.01494	0.16627
C	4.34902	-2.29994	3.47186
H	5.18217	-2.91196	3.19584
H	4.63724	-1.26996	3.44067
H	4.0339	-2.55228	4.46278
C	0.04878	3.3468	1.51314
H	0.85076	3.49195	2.20643
H	0.44729	3.21985	0.52826
H	-0.59593	4.2006	1.5297
C	-2.65532	2.29828	2.78778
H	-3.4534	1.99532	2.14266
H	-2.7725	1.8316	3.74348
H	-2.67572	3.36163	2.9052
C	0.05169	0.73758	3.30986
H	-0.20584	-0.29738	3.2236
H	1.09848	0.86118	3.12587
H	-0.18018	1.08182	4.29608

HypSnPTMS_6 E = -4538.76687777 a.u.

0 1

P	-1.85043	-1.01649	-0.73787
P	1.84998	-1.01834	0.73409
Sn	-0.00029	0.62477	0.00076
Si	-3.8915	-0.13579	0.00267
Si	3.89145	-0.13609	-0.00337
Si	-5.5568	-1.327	-1.25228
Si	-4.16828	-0.37923	2.37046
Si	-3.99342	2.18432	-0.62435
Si	4.16974	-0.37316	-2.37165
Si	3.99346	2.1825	0.62945
Si	5.55598	-1.33037	1.24975
C	-5.26058	-3.21241	-1.22474
H	-6.06135	-3.71689	-1.78019
H	-4.30967	-3.46707	-1.70385
H	-5.25494	-3.61272	-0.20571
C	-7.29119	-0.98753	-0.52444
H	-8.0582	-1.48107	-1.1344
H	-7.37433	-1.37804	0.49597
H	-7.51828	0.08277	-0.4978
C	-5.50263	-0.75469	-3.07158
H	-4.49766	-0.88636	-3.48623
H	-6.20197	-1.34545	-3.67618
H	-5.77825	0.30014	-3.17229
C	-5.61615	0.71815	2.96498
H	-5.42914	1.7774	2.7593
H	-6.55514	0.43845	2.47586
H	-5.75317	0.6052	4.04774
C	-4.56072	-2.18722	2.84566
H	-3.75247	-2.86446	2.55244

H	-4.69311	-2.26878	3.93177
H	-5.48398	-2.5339	2.36861
C	-2.57223	0.16228	3.26416
H	-1.725	-0.47526	2.98771
H	-2.31184	1.19801	3.02149
H	-2.70155	0.09259	4.35144
C	-5.82974	2.69315	-0.77447
H	-5.89936	3.76381	-1.00403
H	-6.33596	2.14516	-1.57602
H	-6.37382	2.51225	0.15837
C	-3.13773	2.46289	-2.30586
H	-3.26815	3.50434	-2.62576
H	-2.06319	2.2611	-2.2439
H	-3.55544	1.81093	-3.07902
C	-3.18347	3.31485	0.68383
H	-3.26626	4.36256	0.36806
H	-3.67404	3.21895	1.65834
H	-2.12062	3.08496	0.81071
C	3.18467	3.31644	-0.6765
H	2.12201	3.0866	-0.8051
H	3.26684	4.36329	-0.35776
H	3.67631	3.22334	-1.65074
C	3.13647	2.45713	2.31097
H	3.26981	3.49689	2.63514
H	2.06136	2.25909	2.24671
H	3.55097	1.80078	3.08214
C	5.82969	2.69077	0.78248
H	5.89906	3.76056	1.01613
H	6.3355	2.1398	1.58224
H	6.37434	2.51345	-0.15071
C	5.50069	-0.76209	3.07026
H	5.77518	0.2928	3.17335
H	4.49572	-0.89562	3.48432
H	6.20043	-1.35347	3.6738
C	7.29089	-0.98945	0.52377
H	7.51797	0.0809	0.49928
H	8.05745	-1.48409	1.1334
H	7.37485	-1.37805	-0.4973
C	5.25971	-3.21568	1.21782
H	6.05999	-3.72141	1.77283
H	4.30839	-3.47141	1.69555
H	5.25492	-3.61377	0.19792
C	5.62113	0.72221	-2.96129
H	6.55907	0.43797	-2.47277
H	5.75833	0.61303	-4.04441
H	5.43705	1.7812	-2.75162
C	4.55728	-2.18081	-2.85199
H	3.74636	-2.85628	-2.56209
H	4.69106	-2.25939	-3.93814
H	5.47866	-2.53196	-2.37458
C	2.57612	0.17582	-3.26504
H	1.72636	-0.4587	-2.98949
H	2.31982	1.21224	-3.02101
H	2.70536	0.107	-4.35237
Si	-1.72958	-3.0071	0.23747
Si	1.72877	-3.00702	-0.24514
C	-0.94892	-2.81577	2.00313
H	-1.60257	-3.24922	2.73098
H	-0.003	-3.31514	2.0309
H	-0.81062	-1.77743	2.22135
C	-3.51101	-3.75875	0.39603
H	-4.21817	-2.97073	0.55045
H	-3.75629	-4.28729	-0.5014
H	-3.5411	-4.43279	1.22648
C	-0.6232	-4.18631	-0.83444
H	-0.15712	-3.6246	-1.61683

H	0.12951	-4.62897	-0.21607
H	-1.23178	-4.95576	-1.26162
C	0.7534	-4.23292	0.89916
H	1.00411	-5.23998	0.63865
H	1.01606	-4.05281	1.92067
H	-0.29792	-4.08209	0.7693
C	0.80746	-2.83629	-1.94386
H	1.32592	-2.13319	-2.56172
H	0.78025	-3.78803	-2.43208
H	-0.19193	-2.4935	-1.77472
C	3.51951	-3.68969	-0.54645
H	4.2048	-2.87157	-0.62366
H	3.80428	-4.31746	0.2719
H	3.53714	-4.25655	-1.45379

HypSnPMe_1 E = -3800.12260562 a.u.

0 1

P	-1.20835	0.25463	0.81366
P	2.15841	-1.5908	0.56386
Sn	-0.28736	-2.16699	0.37117
Si	-3.41478	0.25096	-0.00141
Si	3.60706	0.1435	0.00107
Si	-4.15148	2.45572	0.58086
Si	-3.52776	-0.15804	-2.35538
Si	-4.61096	-1.39978	1.25933
Si	3.57842	0.45969	-2.37242
Si	2.98867	2.09199	1.26793
Si	5.70109	-0.71337	0.81656
C	-2.86682	3.73388	-0.0146
H	-3.19093	4.74752	0.25264
H	-1.8958	3.55368	0.45854
H	-2.72924	3.69643	-1.09987
C	-5.84154	2.85145	-0.21798
H	-6.17427	3.85276	0.08289
H	-5.77941	2.83559	-1.31167
H	-6.61098	2.13507	0.08773
C	-4.29552	2.57942	2.47805
H	-3.35507	2.27922	2.95186
H	-4.51664	3.61117	2.77813
H	-5.09413	1.93739	2.8644
C	-5.33276	-0.5361	-2.85607
H	-5.69631	-1.45395	-2.38116
H	-6.00319	0.281	-2.56891
H	-5.40613	-0.66797	-3.94267
C	-2.92444	1.3677	-3.33004
H	-1.8981	1.63368	-3.05591
H	-2.94335	1.1612	-4.40735
H	-3.5628	2.23757	-3.14276
C	-2.42363	-1.64356	-2.82443
H	-1.36388	-1.39737	-2.68663
H	-2.65573	-2.52927	-2.22379
H	-2.56576	-1.90468	-3.88053
C	-6.46996	-0.96098	1.2632
H	-7.03524	-1.72772	1.8074
H	-6.65323	0.00118	1.75288
H	-6.86972	-0.90643	0.24516
C	-3.96478	-1.43286	3.05273
H	-4.4944	-2.19759	3.63431
H	-2.89418	-1.6605	3.08689
H	-4.11184	-0.46565	3.54291
C	-4.41423	-3.13759	0.49129
H	-4.98468	-3.87025	1.07594
H	-4.78778	-3.16591	-0.53804
H	-3.36691	-3.4581	0.48235
C	1.82226	3.2374	0.28461

H	2.29655	3.60379	-0.63241
H	0.89287	2.72837	0.01385
H	1.56085	4.10863	0.89819
C	2.16192	1.55962	2.89546
H	1.21968	1.03757	2.69772
H	2.80725	0.88772	3.46981
H	1.94086	2.43853	3.514
C	4.57888	3.08625	1.638
H	4.32075	3.99998	2.18779
H	5.28267	2.51468	2.25134
H	5.091	3.38279	0.71625
C	5.64761	-0.75885	2.72159
H	5.55976	0.24553	3.14803
H	4.79206	-1.34922	3.06591
H	6.56216	-1.21644	3.11867
C	7.13507	0.4019	0.2264
H	6.98992	1.44311	0.5302
H	8.08278	0.05288	0.65498
H	7.23208	0.37569	-0.86451
C	6.00528	-2.48484	0.17733
H	6.98032	-2.84343	0.53063
H	5.24065	-3.175	0.54824
H	6.00358	-2.53027	-0.91608
C	4.63381	1.98854	-2.81869
H	5.67364	1.86363	-2.49878
H	4.63104	2.14861	-3.90392
H	4.24188	2.89475	-2.34461
C	4.29114	-1.07599	-3.25119
H	3.7571	-1.98395	-2.95182
H	4.19425	-0.96912	-4.33871
H	5.35267	-1.21343	-3.02012
C	1.78484	0.72581	-2.95746
H	1.16353	-0.13331	-2.68274
H	1.34649	1.62068	-2.50527
H	1.74882	0.83884	-4.04794
C	-0.41063	1.16234	-0.54727
H	-0.76696	2.17118	-0.56023
H	0.64973	1.16042	-0.40398
H	-0.64567	0.68908	-1.47768
C	3.00021	-3.06056	-0.10217
H	3.8096	-2.75363	-0.73113
H	3.38012	-3.65064	0.70554
H	2.30583	-3.6415	-0.67247

HypSnPMe_2 E = -3800.12324666 a.u.

0 1

P	-1.18941	0.15664	-0.74901
P	1.87449	-0.70711	1.47689
Sn	-0.13216	-1.94153	0.36731
Si	-3.41895	0.25429	-0.00564
Si	-4.49205	-1.79534	-0.63884
Si	-3.48372	0.59818	2.36019
Si	-4.28578	2.09783	-1.26393
C	-3.07892	3.56883	-1.13719
H	-3.45762	4.42133	-1.71478
H	-2.94565	3.89297	-0.10011
H	-2.09669	3.29693	-1.53797
C	-5.99552	2.62869	-0.5969
H	-6.4062	3.43775	-1.21374
H	-6.70968	1.79898	-0.61005
H	-5.92256	2.998	0.43196
C	-4.44193	1.58773	-3.09469
H	-4.75806	2.44385	-3.70353
H	-3.47887	1.23433	-3.47774
H	-5.17856	0.7885	-3.22928

C	-5.25456	0.28991	3.00886
H	-5.30907	0.51018	4.08213
H	-5.98456	0.92538	2.4967
H	-5.55607	-0.7533	2.86568
C	-2.96013	2.37995	2.79683
H	-3.67024	3.11504	2.40308
H	-2.91561	2.50396	3.88589
H	-1.96935	2.61255	2.39238
C	-2.28403	-0.61556	3.21439
H	-2.42414	-0.58714	4.30228
H	-2.45259	-1.64716	2.88438
H	-1.24087	-0.34423	3.01309
C	-3.81721	-2.39268	-2.31876
H	-2.74731	-2.61854	-2.25772
H	-4.33833	-3.30449	-2.63609
H	-3.95184	-1.63224	-3.09392
C	-6.37058	-1.47873	-0.7848
H	-6.89125	-2.41456	-1.02271
H	-6.78546	-1.09108	0.15179
H	-6.59498	-0.75904	-1.57914
C	-4.21993	-3.16598	0.66289
H	-4.76803	-4.07019	0.36938
H	-3.16064	-3.4303	0.75184
H	-4.58005	-2.86158	1.65131
Si	3.49355	0.15814	-0.00001
Si	2.81241	2.32861	-0.76194
Si	5.38574	0.37515	1.46413
Si	3.94156	-1.35542	-1.79763
C	5.65188	-1.23239	2.45664
H	6.52803	-1.12641	3.10874
H	4.78559	-1.45105	3.08941
H	5.81959	-2.0923	1.80049
C	5.06688	1.80059	2.69002
H	4.12409	1.64335	3.2244
H	5.87507	1.85633	3.42973
H	5.01073	2.76661	2.17742
C	4.9583	-0.46395	-3.14752
H	5.88291	-0.04392	-2.73801
H	5.23034	-1.16718	-3.94424
H	4.38711	0.35317	-3.60098
C	4.9295	-2.86048	-1.1645
H	4.41003	-3.35503	-0.3368
H	5.06213	-3.59512	-1.96831
H	5.92286	-2.56326	-0.81201
C	2.30576	-1.98065	-2.55743
H	2.49849	-2.50743	-3.50031
H	1.81481	-2.69575	-1.88379
H	1.61026	-1.16029	-2.76192
C	1.75343	2.22136	-2.3438
H	1.44575	3.22814	-2.65376
H	2.32272	1.77806	-3.16835
H	0.84924	1.62212	-2.19547
C	4.3893	3.32425	-1.18327
H	4.99874	2.81042	-1.93437
H	4.11172	4.30509	-1.58912
H	5.01037	3.49232	-0.29712
C	1.85994	3.23132	0.61972
H	1.51009	4.20923	0.2665
H	0.99006	2.65223	0.94516
H	2.49683	3.38978	1.49582
C	6.9647	0.73925	0.45046
H	6.85206	1.63623	-0.16673
H	7.8148	0.89813	1.12574
H	7.21556	-0.09827	-0.20996
C	-0.49686	1.50879	0.25322
H	0.55058	1.5997	0.05446

H	-0.98824	2.42583	0.00323
H	-0.64577	1.29579	1.29117
C	2.7992	-2.20208	1.94844
H	3.32598	-2.57908	1.09681
H	3.49804	-1.96011	2.72172
H	2.11722	-2.94597	2.30402

HypSnPMe_3 E = -3800.12714395 a.u.

0 1

P	1.86512	0.04353	-1.4569
P	-1.87509	-0.15635	-1.39057
Sn	0.06996	-1.36757	-0.21245
Si	3.79206	0.19915	-0.13277
Si	-3.81617	0.16553	-0.13024
Si	5.30605	1.38551	-1.55957
Si	3.37076	1.33845	1.92511
Si	4.54062	-2.05213	0.20845
Si	-4.78857	-2.00771	0.12784
Si	-3.33373	1.23926	1.95332
Si	-5.16499	1.54749	-1.55732
C	4.44711	2.94644	-2.24078
H	5.13138	3.49905	-2.89664
H	3.56219	2.67583	-2.82641
H	4.1307	3.61804	-1.43652
C	6.87352	1.89824	-0.59489
H	7.58347	2.39665	-1.26664
H	6.6336	2.59608	0.21494
H	7.37628	1.02987	-0.15685
C	5.7939	0.26967	-3.0269
H	4.89974	-0.09176	-3.54537
H	6.4019	0.83248	-3.74602
H	6.37645	-0.59878	-2.70093
C	4.84978	1.11115	3.11315
H	4.98787	0.0586	3.38296
H	5.78096	1.46861	2.66095
H	4.68453	1.67677	4.03847
C	3.10719	3.20271	1.61351
H	2.30907	3.37429	0.8835
H	2.82862	3.70925	2.54581
H	4.02033	3.6738	1.2343
C	1.79765	0.63193	2.74337
H	0.91135	0.86508	2.14133
H	1.85965	-0.45443	2.86738
H	1.64844	1.07737	3.73475
C	6.42087	-2.04404	0.54771
H	6.76619	-3.06393	0.75802
H	6.98114	-1.67332	-0.3173
H	6.67389	-1.41854	1.41028
C	4.19019	-3.08603	-1.35363
H	4.56783	-4.10819	-1.22617
H	3.11656	-3.14361	-1.56042
H	4.6715	-2.64818	-2.23327
C	3.66849	-2.86185	1.70268
H	4.04551	-3.8825	1.84432
H	3.85277	-2.30499	2.62777
H	2.58546	-2.9237	1.55072
C	-2.5558	-0.00084	3.17945
H	-3.25936	-0.79983	3.43723
H	-1.65276	-0.46573	2.76838
H	-2.2729	0.51224	4.10694
C	-2.10793	2.67147	1.66405
H	-1.19591	2.31313	1.17432
H	-2.54503	3.44864	1.02936
H	-1.82375	3.13088	2.61875

XC

C	-4.94269	1.92681	2.72016
H	-4.73169	2.39989	3.68715
H	-5.4008	2.68078	2.07104
H	-5.67781	1.13233	2.88616
C	-4.53999	3.35079	-1.49562
H	-4.6687	3.78674	-0.49911
H	-3.47959	3.41379	-1.76172
H	-5.10314	3.96717	-2.20735
C	-6.9833	1.50582	-0.97276
H	-7.07596	1.79806	0.07845
H	-7.58723	2.19894	-1.57141
H	-7.41251	0.50449	-1.08676
C	-5.05374	0.91397	-3.34971
H	-5.61591	1.57278	-4.02317
H	-4.0126	0.8816	-3.68641
H	-5.46143	-0.09742	-3.44015
C	-6.29049	-1.88217	1.30165
H	-7.03053	-1.16282	0.93628
H	-6.78218	-2.8591	1.38722
H	-5.98527	-1.57235	2.3072
C	-5.35724	-2.66189	-1.56978
H	-4.54148	-2.61482	-2.29831
H	-5.68315	-3.70592	-1.48558
H	-6.19652	-2.07756	-1.96136
C	-3.53403	-3.23696	0.87266
H	-2.67592	-3.3844	0.20831
H	-3.15588	-2.89358	1.84069
H	-4.01263	-4.21309	1.02184
C	-1.33032	1.55566	-1.68149
H	-0.91106	1.95437	-0.7814
H	-0.59137	1.56821	-2.45524
H	-2.16826	2.15093	-1.97886
C	1.23243	1.74723	-1.35928
H	0.6313	1.95432	-2.2199
H	0.6397	1.85748	-0.4753
H	2.05432	2.43151	-1.32526

HypSnPMe_4 E = -3800.12735202 a.u.

0 1

P	-1.67042	-0.6074	-0.9293
P	1.67063	-0.60704	0.92986
Sn	0.00006	1.14938	-0.00002
Si	-3.78597	-0.23507	0.01823
Si	3.78606	-0.23508	-0.01814
Si	-5.13624	-1.88801	-1.06903
Si	-3.6925	-0.4964	2.39477
Si	-4.45711	1.97383	-0.62656
Si	3.69209	-0.49754	-2.39454
Si	4.4572	1.97415	0.62553
Si	5.13644	-1.88753	1.06968
C	-4.2394	-3.5703	-1.02414
H	-4.85266	-4.33969	-1.50964
H	-3.28514	-3.5114	-1.558
H	-4.03586	-3.89473	0.00126
C	-6.82927	-2.05181	-0.19891
H	-7.46853	-2.75543	-0.74655
H	-6.71455	-2.43068	0.82269
H	-7.35163	-1.09089	-0.14806
C	-5.39677	-1.38958	-2.89087
H	-4.43261	-1.24715	-3.38997
H	-5.94528	-2.17509	-3.42533
H	-5.96839	-0.45973	-2.97855
C	-5.31211	0.14887	3.17732
H	-5.44696	1.21989	2.99101
H	-6.18566	-0.37618	2.77681

H	-5.29555	-0.00356	4.2636
C	-3.46228	-2.33287	2.85867
H	-2.56625	-2.75023	2.38721
H	-3.34957	-2.4359	3.94504
H	-4.3225	-2.9367	2.551
C	-2.21928	0.48956	3.10151
H	-1.26595	0.03106	2.81305
H	-2.22535	1.53165	2.7636
H	-2.25871	0.49385	4.19806
C	-6.36255	2.08548	-0.55713
H	-6.68989	3.10076	-0.81286
H	-6.82999	1.39392	-1.26612
H	-6.73985	1.85127	0.44387
C	-3.86059	2.33889	-2.39987
H	-4.14088	3.35843	-2.69231
H	-2.77198	2.24924	-2.47708
H	-4.30107	1.64215	-3.11952
C	-3.73441	3.29167	0.55165
H	-4.07435	4.28969	0.24758
H	-4.0553	3.12878	1.58614
H	-2.63916	3.28979	0.52961
C	3.73442	3.29137	-0.55331
H	2.63917	3.28951	-0.53119
H	4.07437	4.28955	-0.24977
H	4.05524	3.12795	-1.58774
C	3.86078	2.3401	2.39868
H	4.14104	3.35981	2.69056
H	2.77218	2.25045	2.47601
H	4.30134	1.64377	3.11867
C	6.36263	2.08583	0.55594
H	6.68994	3.10126	0.81116
H	6.83014	1.39463	1.26525
H	6.73988	1.85116	-0.44496
C	5.39702	-1.38834	2.89131
H	5.96859	-0.45843	2.97857
H	4.43286	-1.24577	3.39037
H	5.94559	-2.1736	3.42608
C	6.82944	-2.05159	0.19956
H	7.35176	-1.09067	0.14834
H	7.46875	-2.75499	0.74742
H	6.71471	-2.43083	-0.82191
C	4.23968	-3.56988	1.02553
H	4.85299	-4.33903	1.51135
H	3.28542	-3.51079	1.55936
H	4.03615	-3.89476	0.00026
C	5.31154	0.14731	-3.17778
H	6.18518	-0.37755	-2.77722
H	5.29472	-0.00566	-4.26398
H	5.44645	1.21842	-2.99205
C	3.46175	-2.33424	-2.85749
H	2.56583	-2.75137	-2.38563
H	3.34879	-2.4378	-3.94378
H	4.32204	-2.93792	-2.54971
C	2.21875	0.48811	-3.10147
H	1.26546	0.02974	-2.8127
H	2.22487	1.53035	-2.76399
H	2.25802	0.49194	-4.19803
C	-1.20105	-2.12917	-0.0482
H	-0.35566	-2.57404	-0.53017
H	-0.95026	-1.89198	0.96459
H	-2.02129	-2.81615	-0.06102
C	1.20114	-2.12911	0.04936
H	0.47991	-2.66774	0.6278
H	0.77912	-1.87581	-0.90072
H	2.06836	-2.73861	-0.09667

SnPHyp2_1 E = -6754.53004675 a.u.

0 1

P	-2.19007	-0.20615	0.21389
P	1.99741	-1.03669	0.03481
Sn	0.06277	0.70214	-0.43621
Si	-3.98325	1.14875	-0.39013
Si	3.9026	0.33444	0.21069
Si	-5.63805	-0.12332	-1.58937
Si	-4.9191	2.29458	1.51713
Si	-3.15908	2.8234	-1.93369
Si	4.53647	1.80674	-1.59151
Si	3.39617	1.65782	2.16906
Si	5.7577	-1.07953	0.79799
C	-6.19731	-1.6865	-0.65162
H	-6.91551	-2.24339	-1.2665
H	-5.35597	-2.35035	-0.43318
H	-6.69088	-1.42989	0.29133
C	-7.19071	0.95935	-1.85527
H	-7.93818	0.39969	-2.43157
H	-7.64739	1.23784	-0.89928
H	-6.96252	1.87861	-2.40142
C	-4.93911	-0.65561	-3.28272
H	-3.9758	-1.16332	-3.16673
H	-5.63262	-1.34639	-3.77801
H	-4.79344	0.20501	-3.944
C	-5.65804	3.9753	0.98062
H	-4.91122	4.6343	0.52752
H	-6.47444	3.8392	0.26314
H	-6.0676	4.48791	1.86027
C	-6.35404	1.32291	2.32133
H	-6.04337	0.33801	2.67785
H	-6.74176	1.88699	3.1791
H	-7.17882	1.18469	1.61364
C	-3.53775	2.59241	2.79421
H	-3.0403	1.6533	3.05653
H	-2.7735	3.26614	2.39252
H	-3.94442	3.04034	3.70918
C	-4.65926	3.69428	-2.73936
H	-4.30344	4.55583	-3.31868
H	-5.18352	3.02471	-3.42933
H	-5.37823	4.05922	-2.00053
C	-2.12374	2.08294	-3.35804
H	-2.04859	2.81771	-4.17004
H	-1.10676	1.84359	-3.03032
H	-2.57279	1.17148	-3.76195
C	-2.11336	4.14902	-1.04233
H	-1.77294	4.89894	-1.76762
H	-2.68715	4.666	-0.26669
H	-1.22802	3.70804	-0.57358
C	2.26601	3.14223	1.74753
H	1.31491	2.8225	1.30543
H	2.03496	3.69952	2.66427
H	2.74247	3.83216	1.04363
C	2.50429	0.58407	3.466
H	2.26135	1.18703	4.35022
H	1.57612	0.16687	3.06527
H	3.12869	-0.25643	3.7834
C	4.98577	2.36005	2.96394
H	4.71436	3.01005	3.80543
H	5.62203	1.55914	3.35428
H	5.57341	2.95236	2.25608
C	5.37586	-2.00132	2.42382
H	5.34883	-1.31459	3.27651
H	4.40626	-2.50634	2.36426
H	6.14693	-2.7559	2.62328

C	7.33263	-0.01874	1.02849
H	7.19017	0.76894	1.77365
H	8.16115	-0.65587	1.36309
H	7.63687	0.45549	0.08897
C	6.14785	-2.37732	-0.54706
H	7.00624	-2.98297	-0.22972
H	5.30355	-3.05307	-0.71096
H	6.40286	-1.90769	-1.50246
C	5.40255	3.34253	-0.84864
H	6.30251	3.06062	-0.29156
H	5.70613	4.02017	-1.65671
H	4.74469	3.89827	-0.17348
C	5.80112	1.00707	-2.77842
H	5.37171	0.17672	-3.3444
H	6.15434	1.75886	-3.49546
H	6.67171	0.63199	-2.23037
C	3.01905	2.38727	-2.5904
H	2.46182	1.53777	-2.99904
H	2.33185	2.96805	-1.9664
H	3.33627	3.01966	-3.42904
Si	-2.54538	-2.03114	1.61876
Si	2.02589	-2.36926	-1.90355
Si	-0.08781	-2.33583	-2.90692
Si	2.48865	-4.55016	-1.1928
Si	3.60008	-1.69815	-3.49953
Si	-0.78067	-2.12647	3.15248
Si	-2.6129	-3.99468	0.34772
Si	-4.54214	-1.75896	2.80808
C	-2.61289	-3.54391	-1.53918
H	-2.5943	-2.48	-1.65172
H	-1.74868	-3.96721	-2.007
H	-3.49569	-3.93589	-1.99953
C	-4.22416	-4.98686	0.77555
H	-4.19677	-5.93895	0.28803
H	-4.28444	-5.12985	1.83423
H	-5.07996	-4.43901	0.44033
C	-1.05764	-5.08118	0.75303
H	-0.84769	-5.72619	-0.07448
H	-0.21565	-4.44579	0.93258
H	-1.25178	-5.67081	1.62455
C	0.05568	-1.59098	-4.69248
H	-0.54189	-0.70588	-4.75879
H	1.07748	-1.34756	-4.89634
H	-0.28941	-2.30868	-5.40712
C	-1.29025	-1.24433	-1.84562
H	-2.27468	-1.66226	-1.87919
H	-0.94799	-1.21878	-0.83216
H	-1.31127	-0.24995	-2.24016
C	-0.78123	-4.14448	-3.01453
H	-1.80318	-4.11645	-3.33034
H	-0.20516	-4.70593	-3.72008
H	-0.71781	-4.6086	-2.05252
C	1.0729	-5.73723	-1.78449
H	1.24522	-6.01824	-2.80245
H	1.06153	-6.61296	-1.16977
H	0.1311	-5.23523	-1.70759
C	4.17818	-5.13173	-1.94835
H	4.92092	-5.16354	-1.17879
H	4.06222	-6.10714	-2.37265
H	4.48326	-4.44529	-2.71033
C	3.59134	-2.94912	-4.9823
H	2.98144	-2.56223	-5.77176
H	4.59083	-3.08692	-5.33858
H	3.19694	-3.88817	-4.65438
C	3.1498	0.07454	-4.14637
H	2.61508	0.60608	-3.38713

H	4.04728	0.60465	-4.38806
H	2.5387	-0.00938	-5.02067
C	5.36417	-1.6635	-2.69308
H	5.34503	-1.04558	-1.81975
H	5.6513	-2.65755	-2.42044
H	6.06918	-1.26826	-3.39426
C	2.59853	-4.58959	0.74368
H	2.03097	-3.77847	1.14972
H	2.20428	-5.51657	1.10449
H	3.62093	-4.49549	1.0449
C	-0.23818	-0.32528	3.62685
H	0.49251	-0.36677	4.40741
H	0.18248	0.15789	2.76983
H	-1.09032	0.22648	3.96496
C	-1.35952	-3.06847	4.74658
H	-0.50309	-3.39175	5.30058
H	-1.95027	-2.414	5.35286
H	-1.94445	-3.91921	4.46551
C	0.71875	-3.06468	2.35554
H	0.60345	-3.08299	1.29193
H	1.62885	-2.56132	2.60703
H	0.75094	-4.0672	2.72812
C	-4.88075	-3.34374	3.87458
H	-4.91149	-3.07679	4.91029
H	-5.81858	-3.77233	3.58873
H	-4.09896	-4.05618	3.71293
C	-4.39554	-0.21466	3.97309
H	-3.7597	0.51602	3.51845
H	-5.36647	0.20631	4.13117
H	-3.97961	-0.51456	4.91222
C	-6.00553	-1.49282	1.5626
H	-5.76355	-0.69368	0.89349
H	-6.16527	-2.39065	1.00288
H	-6.89492	-1.24735	2.10449

SnPHyp2_2 E = -6754.53037974 a.u.

0 1

Sn	0.30526	-0.20757	-0.33498
P	-1.43473	-0.12738	1.54709
P	2.80471	-0.07178	0.73082
Si	-3.65569	-0.66982	0.85974
Si	-0.78663	-0.35853	3.80259
Si	3.64073	2.11109	0.17541
Si	3.63481	-1.93701	-0.53594
Si	-3.68748	-3.05942	0.44985
Si	-4.50956	0.61693	-1.06021
Si	-5.04612	-0.25832	2.80902
Si	2.88455	-3.74506	0.8909
Si	6.04617	-2.17172	-0.44999
Si	2.82921	-2.53317	-2.75773
C	-2.76684	-3.49828	-1.1569
H	-2.80132	-4.58255	-1.32114
H	-3.20649	-3.00566	-2.02767
H	-1.71491	-3.20205	-1.09743
C	-5.47147	-3.73157	0.32492
H	-5.43309	-4.82396	0.22619
H	-6.05693	-3.49915	1.22039
H	-6.0038	-3.33645	-0.5437
C	-2.84137	-3.99336	1.87732
H	-1.80686	-3.66714	2.0056
H	-3.36859	-3.85454	2.82528
H	-2.83441	-5.06679	1.6479
C	-4.67923	-1.56281	4.15836
H	-3.61403	-1.71412	4.33969

H	-5.1455	-1.25142	5.10178
H	-5.11472	-2.52749	3.8757
C	-6.90658	-0.45737	2.44179
H	-7.47007	-0.16596	3.33778
H	-7.24113	0.16846	1.61309
H	-7.16456	-1.49441	2.20799
C	-4.79324	1.50082	3.50147
H	-5.1359	1.54456	4.54264
H	-3.74676	1.80759	3.47336
H	-5.37111	2.22927	2.927
C	3.73359	-3.63645	2.59583
H	3.65868	-2.62196	3.00077
H	3.25216	-4.32716	3.29949
H	4.79354	-3.90379	2.53704
C	1.00163	-3.67037	1.17384
H	0.44395	-3.8058	0.24192
H	0.70297	-4.47607	1.85709
H	0.69259	-2.72076	1.62121
C	3.24117	-5.46161	0.12415
H	4.30902	-5.6431	-0.01922
H	2.85326	-6.23921	0.79481
H	2.7447	-5.58098	-0.84431
C	6.53969	-4.01312	-0.61616
H	7.6309	-4.06985	-0.72294
H	6.2646	-4.58541	0.27524
H	6.09125	-4.49324	-1.48945
C	6.69576	-1.60471	1.24946
H	7.79232	-1.56598	1.24081
H	6.31858	-0.62204	1.53503
H	6.38725	-2.31155	2.02541
C	6.96558	-1.26331	-1.85408
H	6.78386	-0.1879	-1.85278
H	8.04486	-1.42703	-1.73907
H	6.67195	-1.65171	-2.83517
C	2.58935	-1.09071	-3.98137
H	2.00656	-0.27601	-3.54191
H	3.54283	-0.68196	-4.32509
H	2.04305	-1.46147	-4.85808
C	1.16042	-3.46178	-2.68651
H	0.93809	-3.86652	-3.68242
H	1.1746	-4.29779	-1.98157
H	0.33956	-2.79196	-2.41159
C	4.09022	-3.75143	-3.52181
H	3.75128	-4.03707	-4.5259
H	5.08633	-3.30834	-3.61664
H	4.17689	-4.66433	-2.92384
Si	5.7538	2.49901	1.29311
Si	3.84177	2.78326	-2.12711
Si	2.20552	3.73084	1.27296
C	0.34922	3.44315	0.96997
H	-0.21664	4.28853	1.38321
H	0.12453	3.39137	-0.10115
H	-0.02975	2.53188	1.44089
C	2.56162	5.48448	0.59454
H	3.62479	5.73709	0.60037
H	2.18506	5.59659	-0.42776
H	2.03643	6.21493	1.22382
C	2.52859	3.77515	3.15753
H	1.67317	4.23671	3.6668
H	2.67732	2.77651	3.57509
H	3.41525	4.37382	3.39031
C	2.1128	2.88606	-2.92768
H	1.56392	1.94608	-2.81148
H	1.51305	3.68251	-2.47388
H	2.20045	3.09776	-4.00061
C	4.67586	4.49799	-2.27414

H	5.69179	4.48377	-1.86483
H	4.7504	4.76649	-3.33597
H	4.1143	5.2847	-1.76501
C	4.94032	1.58083	-3.1161
H	4.78405	1.72557	-4.19217
H	5.99753	1.76957	-2.90185
H	4.72734	0.53737	-2.87522
C	6.01683	4.37896	1.54035
H	6.05851	4.91307	0.58576
H	5.23506	4.83439	2.15372
H	6.97566	4.53248	2.05256
C	5.74623	1.67803	3.0173
H	6.77054	1.53853	3.38373
H	5.21274	2.31289	3.73253
H	5.24704	0.70465	3.00518
C	7.26833	1.93798	0.27487
H	8.18468	2.20145	0.81849
H	7.28493	0.86357	0.08866
H	7.29458	2.45307	-0.69168
C	-3.30757	0.86509	-2.56263
H	-2.51752	1.52961	-2.28134
H	-2.89428	-0.07955	-2.84855
H	-3.84797	1.28207	-3.38664
C	-4.99663	2.43005	-0.57137
H	-4.24899	2.83787	0.07641
H	-5.06946	3.03015	-1.45425
H	-5.94008	2.42215	-0.06665
C	-6.0788	-0.17012	-1.88582
H	-6.51253	0.53101	-2.56788
H	-5.79665	-1.05566	-2.41601
H	-6.79273	-0.41978	-1.12894
Si	-2.06308	0.88904	5.31581
Si	1.36732	0.55084	3.89825
Si	-0.70719	-2.58252	4.52589
C	2.04953	0.4085	5.70876
H	3.05251	0.77973	5.74219
H	1.43402	0.98408	6.36811
H	2.03833	-0.61681	6.01455
C	1.30472	2.4181	3.37572
H	1.86472	3.00313	4.07503
H	1.72683	2.52944	2.39882
H	0.28808	2.7516	3.3651
C	2.53346	-0.42016	2.68958
H	2.03558	-0.56579	1.75374
H	3.43107	0.14069	2.53257
H	2.77692	-1.37092	3.11581
C	0.02471	-2.65291	6.32115
H	-0.35103	-3.51836	6.82583
H	1.09216	-2.70561	6.26932
H	-0.2633	-1.77357	6.85847
C	0.4186	-3.61238	3.32774
H	0.11203	-4.6374	3.34323
H	0.32698	-3.22769	2.3335
H	1.43772	-3.54006	3.64565
C	-2.49904	-3.32609	4.52845
H	-2.99733	-3.05899	3.62001
H	-2.4428	-4.39191	4.60433
H	-3.04527	-2.93747	5.36242
C	-1.25908	0.78668	7.07839
H	-0.86761	1.74529	7.34806
H	-1.99967	0.49038	7.79157
H	-0.46651	0.06792	7.06769
C	-2.12307	2.74031	4.73892
H	-2.07284	2.7829	3.67095
H	-3.03634	3.18801	5.07117
H	-1.2931	3.27108	5.15647

C	-3.86536	0.17444	5.38466
H	-4.15569	-0.15562	4.40912
H	-3.89587	-0.6514	6.06435
H	-4.53856	0.93618	5.71849

SnPHyp2_3 E = -6754.53188187 a.u.

0 1

P	-2.25232	-0.70364	0.22119
P	1.91137	-0.7189	-0.12319
Sn	-0.02576	0.64799	0.72535
Si	-3.9101	0.95876	0.06287
Si	4.00539	0.29014	0.06053
Si	-6.00665	-0.19094	-0.23975
Si	-4.06522	2.69069	1.74828
Si	-3.33684	1.9097	-2.0797
Si	4.60289	1.34516	-2.02188
Si	3.82064	2.01643	1.74875
Si	5.54481	-1.40112	0.86078
C	-6.72823	-0.88772	1.38633
H	-7.70872	-1.3357	1.18015
H	-6.09078	-1.6671	1.81442
H	-6.86641	-0.10671	2.13941
C	-7.30165	1.02016	-0.95822
H	-8.28068	0.52734	-1.01068
H	-7.41001	1.91574	-0.33686
H	-7.03479	1.33954	-1.97096
C	-5.76792	-1.644	-1.44991
H	-4.91474	-2.26233	-1.15313
H	-6.6664	-2.27343	-1.46771
H	-5.57883	-1.28839	-2.4667
C	-4.41514	4.37516	0.91443
H	-3.58239	4.68768	0.27565
H	-5.32207	4.34748	0.3024
H	-4.5514	5.14196	1.68761
C	-5.49945	2.38062	2.97323
H	-5.36965	1.45039	3.5339
H	-5.54011	3.20614	3.69534
H	-6.46532	2.34084	2.45831
C	-2.45615	2.8829	2.75484
H	-2.15255	1.94249	3.22467
H	-1.62686	3.22485	2.12745
H	-2.60868	3.62446	3.54948
C	-4.48949	3.3402	-2.60652
H	-4.32311	3.56531	-3.66764
H	-5.54529	3.08385	-2.47868
H	-4.29219	4.2509	-2.03406
C	-3.42327	0.55751	-3.42317
H	-2.85524	0.87015	-4.30835
H	-3.00851	-0.38819	-3.06151
H	-4.45802	0.37992	-3.7348
C	-1.55002	2.58978	-2.04128
H	-1.34079	3.13914	-2.96811
H	-1.38632	3.27498	-1.20236
H	-0.81815	1.77462	-1.97761
C	2.77011	3.49727	1.15743
H	1.79644	3.18861	0.76734
H	2.59677	4.17956	1.99938
H	3.29285	4.05737	0.37463
C	3.08161	1.29838	3.35526
H	3.10845	2.05545	4.14905
H	2.04006	0.99182	3.21619
H	3.64512	0.42424	3.69834
C	5.54604	2.72958	2.16215
H	5.41811	3.60549	2.81133
H	6.17252	2.00805	2.69174

H	6.08495	3.05445	1.26696
C	4.54471	-2.80594	1.67098
H	4.01486	-2.43673	2.5554
H	3.79029	-3.21091	0.99082
H	5.21197	-3.61967	1.98152
C	6.731	-0.70669	2.1886
H	6.18847	-0.33839	3.06506
H	7.39904	-1.51086	2.5225
H	7.35172	0.10662	1.79993
C	6.65367	-2.08703	-0.53505
H	7.34698	-2.82851	-0.11833
H	6.07655	-2.57339	-1.32559
H	7.25147	-1.28847	-0.98815
C	6.152	2.43474	-1.76193
H	6.9859	1.85907	-1.34591
H	6.47781	2.85343	-2.72226
H	5.94502	3.27075	-1.08625
C	4.99264	0.1093	-3.42343
H	4.10103	-0.45038	-3.72261
H	5.34696	0.66256	-4.30252
H	5.77015	-0.60633	-3.14021
C	3.14874	2.43623	-2.595
H	2.23168	1.84351	-2.67906
H	2.95411	3.25276	-1.89345
H	3.36595	2.87381	-3.57738
Si	-2.52602	-1.93191	2.20893
Si	1.65567	-2.35988	-1.75601
Si	-0.40691	-2.50618	3.01835
Si	-3.66873	-0.79797	3.90716
Si	-3.67768	-3.89137	1.65232
Si	0.74594	-1.38431	-3.67858
Si	0.20643	-3.99819	-0.92459
Si	3.71336	-3.35053	-2.26601
C	-1.13022	-1.85777	-3.81813
H	-1.59236	-1.26373	-4.57868
H	-1.21879	-2.89355	-4.07153
H	-1.6143	-1.67716	-2.88114
C	0.91964	0.54478	-3.56896
H	1.45605	0.80467	-2.68036
H	1.45184	0.90418	-4.42482
H	-0.05318	0.98949	-3.54124
C	1.69417	-2.03115	-5.24256
H	1.68859	-3.10113	-5.24584
H	1.21238	-1.66925	-6.12676
H	2.70454	-1.67982	-5.2177
C	-1.17855	-3.15582	0.14118
H	-2.09327	-3.13643	-0.41362
H	-1.32097	-3.71142	1.04446
H	-0.88527	-2.15502	0.3805
C	1.20357	-5.24397	0.17874
H	2.14106	-5.46269	-0.28835
H	1.3773	-4.8085	1.14056
H	0.64233	-6.14782	0.29256
C	-0.60724	-4.95304	-2.40439
H	0.12194	-5.58728	-2.86367
H	-1.41943	-5.54775	-2.04165
H	-0.97301	-4.25073	-3.12402
C	3.4779	-4.62306	-3.71129
H	4.06752	-4.32143	-4.55168
H	3.79015	-5.59356	-3.38642
H	2.44615	-4.65606	-3.9929
C	4.39437	-4.27001	-0.69936
H	5.40012	-3.95703	-0.51119
H	3.78317	-4.03389	0.14657
H	4.37541	-5.32625	-0.86937
C	4.97377	-1.97984	-2.8102

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 H                     4.69337  -1.59811  -3.76965
 H                     4.96722  -1.18474  -2.09418
 H                     5.95591  -2.40066  -2.8669
 C                    -2.73701   0.85194   4.32346
 H                    -1.96052   1.01402   3.60534
 H                    -3.42735   1.66888   4.29283
 H                    -2.30928   0.78292   5.30182
 C                    -3.74598  -1.91453   5.49176
 H                    -2.76229  -2.02622   5.89768
 H                    -4.38245  -1.45676   6.21995
 H                    -4.13582  -2.87643   5.23163
 C                    -5.47055  -0.39123   3.31421
 H                    -5.42931   0.13947   2.38601
 H                    -6.01613  -1.30191   3.18045
 H                    -5.96      0.21311   4.04914
 C                    -0.59703  -3.62582   4.5912
 H                     0.24025  -4.28842   4.66066
 H                    -0.63758  -3.00951   5.46494
 H                    -1.49861  -4.19706   4.51551
 C                     0.56547  -0.89391   3.48597
 H                     0.52624  -0.20411   2.66894
 H                     0.1212   -0.44772   4.3511
 H                     1.58527  -1.14065   3.69579
 C                     0.56771  -3.47491   1.64894
 H                     1.46733  -3.87555   2.06735
 H                    -0.03918  -4.27373   1.27683
 H                     0.81252  -2.80976   0.84736
 C                    -2.93558  -5.38239   2.64719
 H                    -1.91678  -5.53305   2.35694
 H                    -2.98022  -5.16962   3.69487
 H                    -3.50043  -6.26685   2.43847
 C                    -5.55473  -3.68695   2.09782
 H                    -5.65419  -3.01228   2.92234
 H                    -6.08158  -3.29681   1.25217
 H                    -5.96371  -4.63902   2.36467
 C                    -3.49751  -4.22928  -0.24951
 H                    -3.08864  -5.20641  -0.40099
 H                    -4.45897  -4.16884  -0.71516
 H                    -2.84553  -3.49896  -0.68133

 HypSnPh_1 E = -4183.44409512  a.u.

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P                    -1.20835   0.25463   0.81366
 P                     2.15841  -1.5908    0.56386
 Sn                   -0.28736  -2.16699   0.37117
 Si                   -3.41478   0.25096  -0.00141
 Si                    3.60706   0.1435    0.00107
 Si                   -4.15148   2.45572   0.58086
 Si                   -3.52776  -0.15804  -2.35538
 Si                   -4.61096  -1.39978   1.25933
 Si                    3.57842   0.45969  -2.37242
 Si                    2.98867   2.09199   1.26793
 Si                    5.70109  -0.71337   0.81656
 C                    -2.86682   3.73388  -0.0146
 H                    -3.19093   4.74752   0.25264
 H                    -1.8958    3.55368   0.45854
 H                    -2.72924   3.69643  -1.09987
 C                    -5.84154   2.85145  -0.21798
 H                    -6.17427   3.85276   0.08289
 H                    -5.77941   2.83559  -1.31167
 H                    -6.61098   2.13507   0.08773
 C                    -4.29552   2.57942   2.47805
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C

C	-5.33276	-0.5361	-2.85607
H	-5.69631	-1.45395	-2.38116
H	-6.00319	0.281	-2.56891
H	-5.40613	-0.66797	-3.94267
C	-2.92444	1.3677	-3.33004
H	-1.8981	1.63368	-3.05591
H	-2.94335	1.1612	-4.40735
H	-3.5628	2.23757	-3.14276
C	-2.42363	-1.64356	-2.82443
H	-1.36388	-1.39737	-2.68663
H	-2.65573	-2.52927	-2.22379
H	-2.56576	-1.90468	-3.88053
C	-6.46996	-0.96098	1.2632
H	-7.03524	-1.72772	1.8074
H	-6.65323	0.00118	1.75288
H	-6.86972	-0.90643	0.24516
C	-3.96478	-1.43286	3.05273
H	-4.4944	-2.19759	3.63431
H	-2.89418	-1.6605	3.08689
H	-4.11184	-0.46565	3.54291
C	-4.41423	-3.13759	0.49129
H	-4.98468	-3.87025	1.07594
H	-4.78778	-3.16591	-0.53804
H	-3.36691	-3.4581	0.48235
C	2.65401	3.59461	0.1412
H	3.54333	3.87145	-0.43551
H	1.83562	3.39904	-0.5575
H	2.37077	4.45809	0.75606
C	1.45121	1.70874	2.31919
H	0.58761	1.49928	1.67906
H	1.61455	0.8388	2.96285
H	1.20298	2.56743	2.95556
C	4.45744	2.55089	2.40212
H	4.21407	3.45851	2.96852
H	4.67904	1.75686	3.12226
H	5.36541	2.75042	1.8228
C	5.64761	-0.75885	2.72159
H	5.55976	0.24553	3.14803
H	4.79206	-1.34922	3.06591
H	6.56216	-1.21644	3.11867
C	7.13507	0.4019	0.2264
H	6.98992	1.44311	0.5302
H	8.08278	0.05288	0.65498
H	7.23208	0.37569	-0.86451
C	6.00528	-2.48484	0.17733
H	6.98032	-2.84343	0.53063
H	5.24065	-3.175	0.54824
H	6.00358	-2.53027	-0.91608
C	4.63381	1.98854	-2.81869
H	5.67364	1.86363	-2.49878
H	4.63104	2.14861	-3.90392
H	4.24188	2.89475	-2.34461
C	4.29114	-1.07599	-3.25119
H	3.7571	-1.98395	-2.95182
H	4.19425	-0.96912	-4.33871
H	5.35267	-1.21343	-3.02012
C	1.78484	0.72581	-2.95746
H	1.16353	-0.13331	-2.68274
H	1.34649	1.62068	-2.50527
H	1.74882	0.83884	-4.04794
C	3.00021	-3.06056	-0.10217
C	3.1035	-3.24028	-1.48139
C	3.54206	-4.00801	0.76729
C	3.74952	-4.36658	-1.99185
H	2.67692	-2.49363	-2.1668
C	4.18749	-5.13426	0.25689

Cl

H	3.46044	-3.86612	1.85472
C	4.29159	-5.31339	-1.12278
H	3.83123	-4.50786	-3.07928
H	4.61462	-5.88115	0.94186
H	4.80063	-6.20124	-1.52493
C	-0.41063	1.16234	-0.54727
C	0.09704	0.46846	-1.64545
C	-0.30657	2.55278	-0.49175
C	0.70782	1.16444	-2.68902
H	0.01486	-0.62723	-1.68965
C	0.30449	3.24848	-1.53488
H	-0.70688	3.09966	0.37426
C	0.81139	2.55432	-2.6338
H	1.10762	0.61722	-3.55496
H	0.38666	4.34431	-1.49143
H	1.29291	3.10301	-3.45612

HypSnPh_2 E = -4183.44691136 a.u.

0 1

P	1.18941	0.15664	0.74901
P	-1.87449	-0.70711	-1.47689
Sn	0.13216	-1.94153	-0.36731
Si	3.41895	0.25429	0.00564
Si	4.49205	-1.79534	0.63884
Si	3.48372	0.59818	-2.36019
Si	4.28578	2.09783	1.26393
C	3.07892	3.56883	1.13719
H	3.45762	4.42133	1.71478
H	2.94565	3.89297	0.10011
H	2.09669	3.29693	1.53797
C	5.99552	2.62869	0.5969
H	6.4062	3.43775	1.21374
H	6.70968	1.79898	0.61005
H	5.92256	2.998	-0.43196
C	4.44193	1.58773	3.09469
H	4.75806	2.44385	3.70353
H	3.47887	1.23433	3.47774
H	5.17856	0.7885	3.22928
C	5.25456	0.28991	-3.00886
H	5.30907	0.51018	-4.08213
H	5.98456	0.92538	-2.4967
H	5.55607	-0.7533	-2.86568
C	2.96013	2.37995	-2.79683
H	3.67024	3.11504	-2.40308
H	2.91561	2.50396	-3.88589
H	1.96935	2.61255	-2.39238
C	2.28403	-0.61556	-3.21439
H	2.42414	-0.58714	-4.30228
H	2.45259	-1.64716	-2.88438
H	1.24087	-0.34423	-3.01309
C	3.81721	-2.39268	2.31876
H	2.74731	-2.61854	2.25772
H	4.33833	-3.30449	2.63609
H	3.95184	-1.63224	3.09392
C	6.37058	-1.47873	0.7848
H	6.89125	-2.41456	1.02271
H	6.78546	-1.09108	-0.15179
H	6.59498	-0.75904	1.57914
C	4.21993	-3.16598	-0.66289
H	4.76803	-4.07019	-0.36938
H	3.16064	-3.4303	-0.75184
H	4.58005	-2.86158	-1.65131
Si	-3.49355	0.15814	0.00001
Si	-2.81241	2.32861	0.76194
Si	-5.38574	0.37515	-1.46413

Si	-3.94156	-1.35542	1.79763
C	-5.65188	-1.23239	-2.45664
H	-6.52803	-1.12641	-3.10874
H	-4.78559	-1.45105	-3.08941
H	-5.81959	-2.0923	-1.80049
C	-5.06688	1.80059	-2.69002
H	-4.12409	1.64335	-3.2244
H	-5.87507	1.85633	-3.42973
H	-5.01073	2.76661	-2.17742
C	-4.9583	-0.46395	3.14752
H	-5.88291	-0.04392	2.73801
H	-5.23034	-1.16718	3.94424
H	-4.38711	0.35317	3.60098
C	-4.9295	-2.86048	1.1645
H	-4.41003	-3.35503	0.3368
H	-5.06213	-3.59512	1.96831
H	-5.92286	-2.56326	0.81201
C	-2.30576	-1.98065	2.55743
H	-2.49849	-2.50743	3.50031
H	-1.81481	-2.69575	1.88379
H	-1.61026	-1.16029	2.76192
C	-1.30425	2.22775	1.92405
H	-1.00979	3.23697	2.23887
H	-1.54122	1.65291	2.82621
H	-0.44104	1.75905	1.44047
C	-4.26203	3.08414	1.75348
H	-4.55348	2.44043	2.59031
H	-3.96342	4.05632	2.16519
H	-5.14325	3.244	1.12328
C	-2.43159	3.4498	-0.73104
H	-2.08099	4.43225	-0.39141
H	-1.65841	3.0109	-1.36941
H	-3.32369	3.59738	-1.34803
C	-6.9647	0.73925	-0.45046
H	-6.85206	1.63623	0.16673
H	-7.8148	0.89813	-1.12574
H	-7.21556	-0.09827	0.20996
C	-2.7992	-2.20208	-1.94844
C	-3.13673	-3.14789	-0.98059
C	-3.17021	-2.40223	-3.27867
C	-3.84628	-4.29348	-1.34203
H	-2.84481	-2.99026	0.06783
C	-3.87918	-3.54779	-3.64003
H	-2.90392	-1.65638	-4.04162
C	-4.21759	-4.49332	-2.6716
H	-4.11268	-5.03883	-0.57873
H	-4.17172	-3.70583	-4.68833
H	-4.77668	-5.39625	-2.95667
C	0.49686	1.50879	-0.25322
C	0.67637	2.83379	0.14351
C	-0.21419	1.21975	-1.41858
C	0.14613	3.87028	-0.62526
H	1.23698	3.06189	1.06162
C	-0.74468	2.25602	-2.18686
H	-0.35564	0.17496	-1.73115
C	-0.56419	3.58141	-1.79041
H	0.28814	4.91487	-0.31255
H	-1.30513	2.02855	-3.10535
H	-0.98232	4.3982	-2.39634

HypSnPh_3 E = -4183.44918205 a.u.

0 1

P	-1.67042	-0.6074	-0.9293
P	1.67063	-0.60704	0.92986
Sn	0.00006	1.14938	-0.00002

Si	-3.78597	-0.23507	0.01823
Si	3.78606	-0.23508	-0.01814
Si	-5.13624	-1.88801	-1.06903
Si	-3.6925	-0.4964	2.39477
Si	-4.45711	1.97383	-0.62656
Si	3.69209	-0.49754	-2.39454
Si	4.4572	1.97415	0.62553
Si	5.13644	-1.88753	1.06968
C	-4.2394	-3.5703	-1.02414
H	-4.85266	-4.33969	-1.50964
H	-3.28514	-3.5114	-1.558
H	-4.03586	-3.89473	0.00126
C	-6.82927	-2.05181	-0.19891
H	-7.46853	-2.75543	-0.74655
H	-6.71455	-2.43068	0.82269
H	-7.35163	-1.09089	-0.14806
C	-5.39677	-1.38958	-2.89087
H	-4.43261	-1.24715	-3.38997
H	-5.94528	-2.17509	-3.42533
H	-5.96839	-0.45973	-2.97855
C	-5.31211	0.14887	3.17732
H	-5.44696	1.21989	2.99101
H	-6.18566	-0.37618	2.77681
H	-5.29555	-0.00356	4.2636
C	-3.46228	-2.33287	2.85867
H	-2.56625	-2.75023	2.38721
H	-3.34957	-2.4359	3.94504
H	-4.3225	-2.9367	2.551
C	-2.21928	0.48956	3.10151
H	-1.26595	0.03106	2.81305
H	-2.22535	1.53165	2.7636
H	-2.25871	0.49385	4.19806
C	-6.36255	2.08548	-0.55713
H	-6.68989	3.10076	-0.81286
H	-6.82999	1.39392	-1.26612
H	-6.73985	1.85127	0.44387
C	-3.86059	2.33889	-2.39987
H	-4.14088	3.35843	-2.69231
H	-2.77198	2.24924	-2.47708
H	-4.30107	1.64215	-3.11952
C	-3.73441	3.29167	0.55165
H	-4.07435	4.28969	0.24758
H	-4.0553	3.12878	1.58614
H	-2.63916	3.28979	0.52961
C	3.73442	3.29137	-0.55331
H	2.63917	3.28951	-0.53119
H	4.07437	4.28955	-0.24977
H	4.05524	3.12795	-1.58774
C	3.86078	2.3401	2.39868
H	4.14104	3.35981	2.69056
H	2.77218	2.25045	2.47601
H	4.30134	1.64377	3.11867
C	6.36263	2.08583	0.55594
H	6.68994	3.10126	0.81116
H	6.83014	1.39463	1.26525
H	6.73988	1.85116	-0.44496
C	5.39702	-1.38834	2.89131
H	5.96859	-0.45843	2.97857
H	4.43286	-1.24577	3.39037
H	5.94559	-2.1736	3.42608
C	6.82944	-2.05159	0.19956
H	7.35176	-1.09067	0.14834
H	7.46875	-2.75499	0.74742
H	6.71471	-2.43083	-0.82191
C	4.23968	-3.56988	1.02553
H	4.85299	-4.33903	1.51135

CIV

H	3.28542	-3.51079	1.55936
H	4.03615	-3.89476	0.00026
C	5.31154	0.14731	-3.17778
H	6.18518	-0.37755	-2.77722
H	5.29472	-0.00566	-4.26398
H	5.44645	1.21842	-2.99205
C	3.46175	-2.33424	-2.85749
H	2.56583	-2.75137	-2.38563
H	3.34879	-2.4378	-3.94378
H	4.32204	-2.93792	-2.54971
C	2.21875	0.48811	-3.10147
H	1.26546	0.02974	-2.8127
H	2.22487	1.53035	-2.76399
H	2.25802	0.49194	-4.19803
C	-1.20105	-2.12917	-0.0482
C	-0.50239	-2.0506	1.15634
C	-1.53993	-3.37479	-0.57812
C	-0.14333	-3.21717	1.83209
H	-0.23552	-1.06913	1.57436
C	-1.18051	-4.54105	0.09729
H	-2.09076	-3.43649	-1.5279
C	-0.4825	-4.46226	1.30268
H	0.40712	-3.155	2.78198
H	-1.44743	-5.5229	-0.32009
H	-0.19942	-5.38181	1.83506
C	1.20114	-2.12911	0.04936
C	0.76471	-2.06331	-1.27368
C	1.27747	-3.36213	0.69824
C	0.40559	-3.23022	-1.94882
H	0.7048	-1.09182	-1.7854
C	0.91797	-4.52867	0.02335
H	1.62156	-3.41376	1.74142
C	0.48237	-4.46279	-1.3004
H	0.06195	-3.17818	-2.99205
H	0.97801	-5.50059	0.53447
H	0.19919	-5.38258	-1.83231

HypSnPh_4 E = -4183.44929007 a.u.

0 1

Sn	0.00001	-0.51584	0.00015
P	2.00438	1.13466	-0.00754
P	-2.00435	1.1347	0.00744
Si	3.83009	-0.33866	0.16152
Si	-3.83013	-0.33857	-0.16138
Si	3.72982	-2.3936	-1.10107
Si	3.77646	-0.85884	2.51201
Si	5.9112	0.7924	-0.25958
Si	-3.77653	-0.85887	-2.51188
Si	-5.91132	0.79231	0.25972
Si	-3.72965	-2.39361	1.10104
C	2.01348	-1.34244	3.06695
H	2.02943	-1.66362	4.11631
H	1.33609	-0.48318	2.99629
H	1.6041	-2.16496	2.47075
C	4.94712	-2.31642	2.91097
H	5.9714	-2.11356	2.5828
H	4.96834	-2.49193	3.99384
H	4.61513	-3.24206	2.42896
C	4.30736	0.66407	3.53034
H	3.75971	1.5548	3.20586
H	4.09813	0.49953	4.59473
H	5.37903	0.86372	3.42571
C	2.62219	-3.69646	-0.24891
H	2.66357	-4.63783	-0.81166
H	2.9539	-3.9019	0.77408

H	1.57801	-3.37019	-0.20901
C	5.48611	-3.14066	-1.22325
H	5.44089	-4.09389	-1.76496
H	6.17366	-2.48121	-1.76296
H	5.90762	-3.33665	-0.23186
C	3.06702	-2.10853	-2.86461
H	2.08609	-1.62312	-2.84338
H	3.7429	-1.4778	-3.45105
H	2.9602	-3.06862	-3.38453
C	6.22774	0.95112	-2.13777
H	5.42116	1.48468	-2.64948
H	7.16266	1.49583	-2.31913
H	6.32091	-0.03779	-2.60014
C	7.35102	-0.21982	0.48671
H	8.30389	0.27128	0.25159
H	7.26925	-0.28175	1.57704
H	7.38871	-1.238	0.08899
C	5.93214	2.50872	0.57157
H	6.78617	3.0959	0.21146
H	5.01807	3.07288	0.37445
H	6.02691	2.40208	1.65664
C	-4.3076	0.66388	-3.53037
H	-3.76039	1.55482	-3.20573
H	-4.09795	0.49938	-4.59468
H	-5.37939	0.86312	-3.42611
C	-2.01348	-1.34232	-3.06674
H	-1.60392	-2.16457	-2.4703
H	-2.02943	-1.66386	-4.11599
H	-1.33625	-0.48291	-2.99638
C	-4.94703	-2.31657	-2.91084
H	-5.97132	-2.11388	-2.58257
H	-4.96833	-2.49195	-3.99374
H	-4.6149	-3.24223	-2.42898
C	-7.35101	-0.22021	-0.48643
H	-8.30396	0.2707	-0.25118
H	-7.26937	-0.28211	-1.57676
H	-7.38845	-1.2384	-0.08871
C	-5.9326	2.50848	-0.57168
H	-6.78758	3.09498	-0.21271
H	-5.01926	3.07345	-0.37347
H	-6.0259	2.40163	-1.65685
C	-6.22791	0.95122	2.13789
H	-5.42143	1.48498	2.64957
H	-7.16292	1.4958	2.31916
H	-6.32092	-0.03766	2.60036
C	-3.06691	-2.10869	2.86463
H	-2.0864	-1.62243	2.84358
H	-3.74333	-1.47876	3.4513
H	-2.95928	-3.06889	3.38418
C	-2.62204	-3.69638	0.24869
H	-2.66378	-4.63793	0.8111
H	-2.95352	-3.90138	-0.77446
H	-1.57778	-3.37031	0.20918
C	-5.48588	-3.14083	1.22326
H	-5.44051	-4.09408	1.76493
H	-6.17347	-2.48149	1.76306
H	-5.90743	-3.33681	0.23189
C	1.97548	2.18851	-1.49111
C	2.13489	1.61931	-2.75437
C	1.79419	3.56631	-1.36461
C	2.11193	2.42714	-3.89162
H	2.2774	0.53353	-2.85439
C	1.77172	4.37395	-2.50161
H	1.66858	4.01489	-0.36847
C	1.9302	3.80429	-3.76525
H	2.23718	1.97812	-4.88753

H	1.62887	5.45985	-2.40225
H	1.91226	4.44116	-4.66147
C	-1.97541	2.18881	1.49082
C	-2.0129	1.60965	2.75905
C	-1.91608	3.57675	1.35924
C	-1.98991	2.41775	3.89611
H	-2.05929	0.51591	2.86306
C	-1.89357	4.38461	2.49607
H	-1.88658	4.03317	0.35918
C	-1.93009	3.80508	3.76462
H	-2.01903	1.96092	4.89591
H	-1.84683	5.47851	2.3927
H	-1.91214	4.44215	4.6607

HypSnPh_5 E = -4183.44931396 a.u.

0 1

P	1.86512	0.04353	-1.4569
P	-2.13861	-0.42755	-1.14883
Sn	0.06996	-1.36757	-0.21245
Si	3.79206	0.19915	-0.13277
Si	-3.9435	-0.34083	0.33261
Si	5.30605	1.38551	-1.55957
Si	3.37076	1.33845	1.92511
Si	4.54062	-2.05213	0.20845
Si	-4.59317	-2.61704	0.69582
Si	-3.36109	0.80964	2.34858
Si	-5.61591	0.84156	-0.92066
C	4.44711	2.94644	-2.24078
H	5.13138	3.49905	-2.89664
H	3.56219	2.67583	-2.82641
H	4.1307	3.61804	-1.43652
C	6.87352	1.89824	-0.59489
H	7.58347	2.39665	-1.26664
H	6.6336	2.59608	0.21494
H	7.37628	1.02987	-0.15685
C	5.7939	0.26967	-3.0269
H	4.89974	-0.09176	-3.54537
H	6.4019	0.83248	-3.74602
H	6.37645	-0.59878	-2.70093
C	4.84978	1.11115	3.11315
H	4.98787	0.0586	3.38296
H	5.78096	1.46861	2.66095
H	4.68453	1.67677	4.03847
C	3.10719	3.20271	1.61351
H	2.30907	3.37429	0.8835
H	2.82862	3.70925	2.54581
H	4.02033	3.6738	1.2343
C	1.79765	0.63193	2.74337
H	0.91135	0.86508	2.14133
H	1.85965	-0.45443	2.86738
H	1.64844	1.07737	3.73475
C	6.42087	-2.04404	0.54771
H	6.76619	-3.06393	0.75802
H	6.98114	-1.67332	-0.3173
H	6.67389	-1.41854	1.41028
C	4.19019	-3.08603	-1.35363
H	4.56783	-4.10819	-1.22617
H	3.11656	-3.14361	-1.56042
H	4.6715	-2.64818	-2.23327
C	3.66849	-2.86185	1.70268
H	4.04551	-3.8825	1.84432
H	3.85277	-2.30499	2.62777
H	2.58546	-2.9237	1.55072
C	-2.29263	-0.30705	3.47009
H	-2.85317	-1.18607	3.80616

H	-1.39211	-0.65792	2.95381
H	-1.97074	0.24858	4.35957
C	-2.37084	2.3828	1.92191
H	-1.48433	2.13783	1.32685
H	-2.97509	3.0906	1.34591
H	-2.03765	2.88567	2.83808
C	-4.94353	1.2956	3.30212
H	-4.68271	1.80286	4.23917
H	-5.56721	1.97754	2.71419
H	-5.54651	0.41597	3.55079
C	-5.22359	2.71035	-0.92668
H	-5.28912	3.13787	0.07959
H	-4.21853	2.90474	-1.31567
H	-5.94047	3.24173	-1.56489
C	-7.33273	0.57552	-0.12602
H	-7.33798	0.86574	0.9298
H	-8.08632	1.17914	-0.64687
H	-7.64086	-0.47356	-0.19218
C	-5.63571	0.20664	-2.71589
H	-6.35256	0.78068	-3.31607
H	-4.64574	0.30319	-3.17307
H	-5.9186	-0.84939	-2.76123
C	-5.95062	-2.67014	2.03889
H	-6.81424	-2.05514	1.76583
H	-6.29998	-3.70066	2.17837
H	-5.57163	-2.31237	3.00256
C	-5.26882	-3.3579	-0.92525
H	-4.55693	-3.21581	-1.74467
H	-5.4465	-4.43389	-0.80691
H	-6.21599	-2.88975	-1.21312
C	-3.11317	-3.66787	1.28324
H	-2.32719	-3.71255	0.52187
H	-2.67105	-3.26795	2.20117
H	-3.44228	-4.69519	1.48433
C	-1.85501	1.3364	-1.49588
C	-1.87648	2.26444	-0.45496
C	-1.61643	1.76046	-2.80373
C	-1.65828	3.61651	-0.72099
H	-2.0641	1.93051	0.57583
C	-1.39876	3.11229	-3.06968
H	-1.5996	1.02856	-3.62429
C	-1.41929	4.04035	-2.02819
H	-1.6748	4.34797	0.09989
H	-1.21071	3.44681	-4.10031
H	-1.24747	5.10598	-2.23807
C	1.23243	1.74723	-1.35928
C	1.04207	2.35057	-0.11632
C	0.93737	2.44982	-2.52827
C	0.55782	3.65686	-0.04161
H	1.27485	1.79728	0.80505
C	0.45279	3.75562	-2.45349
H	1.08749	1.97387	-3.50819
C	0.26337	4.35935	-1.21009
H	0.40823	4.13252	0.93845
H	0.22015	4.30961	-3.37461
H	-0.11848	5.38886	-1.15139

SnHyp2_TS E = -4538.76424152 a.u.

0 1

Sn	-0.01853700	0.39426700	-0.73255100
P	-2.04279100	-1.17217500	-0.03862400
P	1.91283500	-0.74883700	0.41256100
Si	-3.78581400	0.38911600	0.24069400
Si	-2.29518100	-2.44098800	-2.00303500
Si	1.75283100	-2.44699600	2.00600400

Si	3.91370900	0.33317100	-0.12566700
Si	-3.96476000	2.36809700	-1.12906300
Si	-3.31382700	1.11652500	2.48509800
Si	-5.86968900	-0.80892800	0.30516200
Si	4.21748000	0.18704400	-2.50923800
Si	5.85736000	-0.60539600	0.94599200
Si	3.64970500	2.62514500	0.58473400
C	-1.49138000	1.66956200	2.62403700
H	-1.28971200	2.05325500	3.63234300
H	-0.81271800	0.82786300	2.44687500
H	-1.25011300	2.46515800	1.91058700
C	-4.42251900	2.58987000	2.99153800
H	-5.48606400	2.34883100	2.89601200
H	-4.22949400	2.85601500	4.03847200
H	-4.21917800	3.47513500	2.37942100
C	-3.59533500	-0.31492500	3.71426700
H	-3.07370900	-1.21841000	3.38250800
H	-3.21644400	-0.04107300	4.70691200
H	-4.65975900	-0.55244800	3.81471200
C	-2.61949900	3.64475600	-0.66817200
H	-2.76478800	4.56141300	-1.25392300
H	-2.66441700	3.91328100	0.39228900
H	-1.61474200	3.26457700	-0.88163300
C	-5.66574400	3.17007300	-0.77746800
H	-5.72816100	4.13795400	-1.29101500
H	-6.48754700	2.54465400	-1.14247800
H	-5.81871400	3.34445700	0.29200800
C	-3.85207800	2.04878300	-3.00476000
H	-2.87354600	1.64980000	-3.28729800
H	-4.61649600	1.34230800	-3.34269500
H	-4.00123800	2.99305200	-3.54360800
C	-6.55396400	-1.11216400	-1.45343000
H	-5.86336800	-1.69778100	-2.06744400
H	-7.50230600	-1.66109300	-1.39592400
H	-6.74506000	-0.16488600	-1.96982500
C	-7.18122400	0.19649400	1.26655200
H	-8.14549100	-0.32622000	1.22933700
H	-6.90248700	0.30586900	2.32002800
H	-7.32241000	1.19624000	0.84554900
C	-5.62287800	-2.47165700	1.20582300
H	-6.47486000	-3.13922400	1.02674100
H	-4.70987400	-2.97448300	0.87607900
H	-5.53721600	-2.31108100	2.28520800
C	-0.56823400	-3.13429900	-2.41333300
H	0.12205000	-2.35270300	-2.74835200
H	-0.12016500	-3.62062300	-1.54260300
H	-0.65230600	-3.87682800	-3.21702500
C	-3.44290100	-3.91255100	-1.63016000
H	-3.08859400	-4.46083100	-0.75161300
H	-4.47317800	-3.59945800	-1.44107700
H	-3.44949500	-4.60103300	-2.48477100
C	-2.93461000	-1.49270400	-3.52232500
H	-3.88936000	-0.99964200	-3.32269400
H	-2.21915700	-0.72506100	-3.83419400
H	-3.07600900	-2.18502700	-4.36222200
C	4.72916400	-1.58141700	-3.00814600
H	3.99888600	-2.31123600	-2.64310200
H	4.77619900	-1.66488000	-4.10111800
H	5.70963200	-1.85286500	-2.60521000
C	2.64094700	0.62721000	-3.48665800
H	2.22523400	1.59600700	-3.19424600
H	2.87777700	0.66580600	-4.55773400
H	1.86593300	-0.13368900	-3.34518100
C	5.58563800	1.41968000	-3.02286800
H	6.52542700	1.23099700	-2.49534100
H	5.77978300	1.33564400	-4.09941600

H	5.28490000	2.45286600	-2.81704700
C	7.41085900	0.39390300	0.45285700
H	8.28771200	-0.04934500	0.94250600
H	7.58267000	0.35822300	-0.62778100
H	7.35119600	1.44279100	0.75338600
C	6.19090700	-2.40317700	0.38630700
H	6.69233800	-2.96679700	1.18216000
H	5.27892000	-2.93740400	0.11432800
H	6.85112900	-2.39925800	-0.48786400
C	5.67461500	-0.48789500	2.84357200
H	4.72811900	-0.90596300	3.19745500
H	6.49306300	-1.02350800	3.34012500
H	5.71531800	0.55901800	3.16427000
C	3.30059200	-3.54610500	2.10174300
H	3.48071400	-4.05668800	1.15133100
H	4.20351500	-2.99872000	2.37771300
H	3.12468000	-4.31406400	2.86653200
C	0.28797800	-3.55925700	1.54894300
H	-0.61640200	-2.97716600	1.34647000
H	0.51958200	-4.15946400	0.66331600
H	0.08574200	-4.24590200	2.38137300
C	1.45175200	-1.61741200	3.69176000
H	1.39575100	-2.37342200	4.48519100
H	2.25378300	-0.91548000	3.93976500
H	0.50953600	-1.06100000	3.68170800
C	2.80488900	2.65777700	2.29189300
H	1.83795700	2.14642600	2.26179300
H	3.42282400	2.15772100	3.04546100
H	2.63969400	3.69252300	2.61711300
C	2.60063000	3.61001000	-0.66960800
H	2.44013500	4.63056700	-0.29980500
H	3.10478100	3.67856000	-1.63989100
H	1.61987800	3.15002600	-0.82961000
C	5.33761100	3.51068900	0.72937400
H	5.17036600	4.57582600	0.93346700
H	5.93381200	3.10428100	1.55292100
H	5.92505500	3.43292600	-0.19119600

SnPHyp_min E = -4538.76661068 a.u.

0 1

Sn	0.00918700	0.42825700	-0.59292400
P	-2.03197900	-1.15584500	-0.05152900
P	1.97716000	-1.06563400	0.05520900
Si	-3.79729300	0.37901500	0.20807300
Si	-2.24966900	-2.45760100	-1.99665600
Si	1.78828400	-2.46863600	1.91722200
Si	3.87307500	0.30358700	-0.13174800
Si	-3.97898600	2.35533100	-1.16433800
Si	-3.35270800	1.11216200	2.45644200
Si	-5.86887100	-0.84065400	0.26457800
Si	4.17702900	0.55242400	-2.50803300
Si	5.87358400	-0.71868000	0.73606800
Si	3.58907000	2.46728500	0.89998200
C	-1.52088000	1.63364500	2.61353400
H	-1.32364800	2.02837700	3.61827600
H	-0.86224300	0.76973400	2.46462500
H	-1.25239900	2.41257700	1.89121000
C	-4.43965500	2.60733800	2.94391200
H	-5.50626800	2.37961700	2.84917200
H	-4.24512500	2.88227500	3.98820700
H	-4.22362100	3.48257200	2.32210700
C	-3.66445100	-0.30499200	3.69460600
H	-3.15421100	-1.21897500	3.37420300
H	-3.28813600	-0.02889000	4.68761100
H	-4.73297600	-0.52541600	3.79006700

CX

C	-2.64377400	3.63958900	-0.69597700
H	-2.79542900	4.55805000	-1.27726600
H	-2.69152600	3.90301200	0.36567500
H	-1.63651500	3.26696100	-0.90988400
C	-5.68680200	3.14914100	-0.82756300
H	-5.74930600	4.11603500	-1.34298600
H	-6.50291600	2.51989800	-1.19864400
H	-5.84961100	3.32464500	0.24031800
C	-3.84926600	2.02847800	-3.03741700
H	-2.86820500	1.62821000	-3.30867600
H	-4.61016000	1.32028400	-3.37969400
H	-3.99299600	2.97034800	-3.58185500
C	-6.53214000	-1.17597600	-1.49603900
H	-5.84682200	-1.79773700	-2.08010500
H	-7.49497600	-1.69898100	-1.43825400
H	-6.69033800	-0.24051000	-2.04388300
C	-7.19600900	0.16965700	1.19904300
H	-8.14984600	-0.37288900	1.18326200
H	-6.91606000	0.31956700	2.24720100
H	-7.35853100	1.15197800	0.74575500
C	-5.61870600	-2.48833500	1.19107900
H	-6.46420300	-3.16407700	1.01201600
H	-4.69918500	-2.98948200	0.87761600
H	-5.54582400	-2.31227800	2.26889400
C	-0.51854100	-3.12743100	-2.41652000
H	0.11535700	-2.36192400	-2.87535900
H	0.00395500	-3.49133100	-1.52765000
H	-0.61226200	-3.95891500	-3.12671600
C	-3.38069200	-3.93506600	-1.59844400
H	-3.01879200	-4.46675100	-0.71286500
H	-4.41415900	-3.63026200	-1.41281100
H	-3.38064200	-4.63566300	-2.44320400
C	-2.91767200	-1.52183300	-3.51123000
H	-3.88233000	-1.04984900	-3.30789800
H	-2.21944900	-0.73895300	-3.82369900
H	-3.04689100	-2.21603500	-4.35155000
C	4.90731700	-1.04697400	-3.24895200
H	4.31374700	-1.91858800	-2.95465800
H	4.90735400	-0.98699100	-4.34451100
H	5.93926400	-1.21000800	-2.92132800
C	2.53265000	0.90826900	-3.40710500
H	2.01891100	1.78477800	-2.99952300
H	2.72921600	1.09318100	-4.47099000
H	1.85804900	0.04790500	-3.33705200
C	5.36853500	2.00507000	-2.86233700
H	6.33608100	1.87068700	-2.36880000
H	5.54886600	2.08170200	-3.94198100
H	4.94643700	2.95825500	-2.52631400
C	7.38986600	0.28976000	0.15319000
H	8.30132500	-0.14743000	0.58068300
H	7.48884600	0.26172400	-0.93698100
H	7.33921200	1.33636700	0.46479900
C	6.11407000	-2.49473400	0.08004300
H	6.82695600	-3.03959300	0.71126100
H	5.18137600	-3.06093700	0.04966000
H	6.51815900	-2.46540100	-0.93687600
C	5.86743400	-0.69159100	2.64678700
H	4.99631500	-1.20014900	3.06986800
H	6.76865300	-1.18316100	3.03383500
H	5.86312400	0.33985300	3.01620300
C	3.26475800	-3.66146700	2.03125500
H	3.37161400	-4.23210000	1.10380600
H	4.21191800	-3.15983900	2.23864600
H	3.07381600	-4.37314400	2.84507600
C	0.22980100	-3.51925300	1.66923700
H	-0.65497000	-2.90374900	1.47821200

H	0.35717900	-4.20687900	0.82680700
H	0.05334700	-4.11861400	2.57194100
C	1.65741600	-1.45000300	3.51747300
H	1.64123500	-2.11534500	4.39003600
H	2.50192400	-0.76319800	3.62472300
H	0.73757800	-0.85703700	3.52400600
C	2.74146200	2.29081700	2.59807900
H	1.77164200	1.79112700	2.51128800
H	3.35924200	1.70690200	3.28848300
H	2.57695100	3.28024700	3.04260100
C	2.55454100	3.64140600	-0.19508200
H	2.43967900	4.60957900	0.30884500
H	3.04197800	3.82053900	-1.15941700
H	1.55470300	3.24153200	-0.39225100
C	5.29092700	3.29950900	1.16124700
H	5.14400400	4.31053100	1.56187200
H	5.90905400	2.74487900	1.87491800
H	5.84608200	3.38709000	0.22173500

(PH2)2Ge_1 E = -688.85136065 a.u.

0 1

P	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.43236899
H	1.41837197	0.00000000	-0.20377932
P	0.88991018	-2.60705885	-2.25469668
H	0.12239807	-3.19949288	-3.30886711
H	1.13322713	-1.33540386	-2.86843377
Ge	-0.77221463	-2.23741584	-0.52870777

(PH2)2Ge_2 E = -688.85041933 a.u.

0 1

P	-1.78106100	0.78724100	-0.11622600
H	-2.81636300	0.11921200	0.61581600
H	-1.47610300	1.79824300	0.85334400
P	1.78101200	0.78724600	-0.11622600
H	1.47611500	1.79862500	0.85295700
H	2.81629600	0.11940700	0.61600100
Ge	0.00002500	-0.85790000	0.01714600

(PMe2)2Ge_1 E = -846.07873894 a.u.

0 1

P	-1.63766000	0.73883200	-0.35182700
P	1.75890400	0.19947100	-0.18797400
C	-3.15210100	-0.29837700	-0.85073500
H	-4.02726100	0.35642700	-0.90563400
H	-2.98442300	-0.72567200	-1.84300100
H	-3.36406500	-1.10980800	-0.14727800
C	1.85074100	2.04772300	-0.45288000
H	2.58164200	2.27676200	-1.23325200
H	0.86517200	2.39335300	-0.77204300
H	2.13268500	2.56116500	0.47026600
Ge	-0.06479500	-1.15345700	0.11506300
C	-2.13175200	1.12388000	1.44927900
H	-1.29456300	1.61041700	1.95648500
H	-2.97796900	1.81817400	1.43753000
H	-2.41894300	0.23255100	2.01595700
C	3.47938900	-0.38232100	0.25556600
H	3.45471900	-1.46044600	0.42788200
H	4.17395400	-0.17398300	-0.56266300
H	3.83615500	0.11171700	1.16337600

(PMe2)2Ge_4 E = -846.07873894 a.u.

0 1

P	1.72982100	0.43371700	0.47489100
P	-1.72985400	0.43409700	-0.47516100
C	3.33643800	-0.48500200	0.07664300
H	4.18730500	0.12335100	0.39528800
H	3.36035800	-1.42508800	0.63361100
H	3.43392200	-0.70363000	-0.99028900
C	-1.76953200	1.82491800	0.81138900
H	-2.04746500	1.44202700	1.79678800
H	-0.78661800	2.29305400	0.88723200
H	-2.49736800	2.57957300	0.50103400
Ge	-0.00010700	-1.17858200	-0.00001900
C	1.76964500	1.82498400	-0.81112400
H	0.78694600	2.29369600	-0.88618500
H	2.49803700	2.57911400	-0.50077300
H	2.04687400	1.44244400	-1.79684800
C	-3.33614200	-0.48510100	-0.07646000
H	-4.18729700	0.12325700	-0.39434500
H	-3.36019100	-1.42488600	-0.63393500
H	-3.43303700	-0.70429300	0.99040600

(PtBu2)2Ge_1 E = -1317.63999875 a.u.

0 1

P	1.80684800	0.48907900	0.34351900
P	-1.86234700	0.10208800	-0.19918400
C	2.89910100	-0.82474200	1.30085400
C	-2.15826600	1.68651300	0.88972100
Ge	0.07530200	-1.13790300	-0.48446900
C	2.65962200	0.96372200	-1.35921300
C	-3.45178000	-0.97417000	-0.47749100
C	3.53301800	-1.93797100	0.45194200
H	4.04431100	-2.65608900	1.10895900
H	2.78104400	-2.48979500	-0.12365600
H	4.27805300	-1.54358500	-0.24500200
C	1.94657200	-1.46087900	2.33629100
H	2.51945900	-2.09114400	3.02936100
H	1.42377500	-0.69780700	2.92391900
H	1.19276800	-2.10347400	1.86040400
C	3.99685600	-0.06089100	2.07007600
H	3.55971500	0.71182900	2.71072100
H	4.55909100	-0.75934800	2.70584300
H	4.70727400	0.42460100	1.39631600
C	4.08655500	1.48087000	-1.09617900
H	4.09907600	2.23557400	-0.30252500
H	4.76932900	0.67302200	-0.81546000
H	4.48111000	1.94370200	-2.01141500
C	2.70203000	-0.14282000	-2.42835500
H	1.69422200	-0.45427600	-2.72917400
H	3.20838700	0.23658600	-3.32767900
H	3.24022300	-1.03132800	-2.09177000
C	1.80300800	2.13067300	-1.89433400
H	2.20722000	2.47393000	-2.85617700
H	0.76213300	1.82574100	-2.05430400
H	1.80575300	2.97592900	-1.19858600
C	-1.12519200	2.74139100	0.45029300
H	-1.25701100	3.64300600	1.06390100
H	-0.10250000	2.38157600	0.58764200
H	-1.26153300	3.01823800	-0.59998400
C	-3.56543200	2.27687100	0.68998100
H	-4.36049000	1.60607100	1.02474100
H	-3.63903300	3.19617100	1.28589400
H	-3.74428000	2.54233100	-0.35615500
C	-1.93256100	1.33173800	2.37363000
H	-2.08260100	2.22851500	2.99103700
H	-2.62684100	0.56033600	2.71970400

H	-0.91129000	0.97392100	2.53348400
C	-4.13194100	-1.32382800	0.86135400
H	-4.49230100	-0.43825900	1.39151600
H	-4.99947000	-1.96995400	0.66927100
H	-3.44483900	-1.86178500	1.52197100
C	-4.43885000	-0.25246900	-1.41884400
H	-5.28356400	-0.92009200	-1.63613800
H	-4.84224900	0.66135300	-0.98027900
H	-3.95587600	0.00658800	-2.36608900
C	-3.01418400	-2.28390500	-1.16270600
H	-3.90861000	-2.87975800	-1.38676200
H	-2.48966800	-2.09500500	-2.10509500
H	-2.35931500	-2.88253100	-0.52257400

(PtBu2)2Ge_4 E = -1317.63991675 a.u.

0 1

P	-1.79310200	0.57849700	0.03312100
P	1.86949400	0.01497400	-0.25635900
C	-2.83201100	0.13160300	-1.56524400
C	2.14247800	1.91234300	0.07425900
Ge	-0.06998200	-1.24656800	-0.13269400
C	-2.72631100	-0.04808500	1.63955400
C	3.46097000	-1.06904200	-0.03323900
C	-4.14324200	0.55388800	1.67939600
H	-4.80703900	0.08662300	0.94557800
H	-4.58265200	0.39036200	2.67325200
H	-4.12371100	1.63244200	1.49016300
C	-2.80818500	-1.57355100	1.83304900
H	-3.36089300	-1.79803600	2.75665100
H	-3.31861500	-2.07451300	1.00784000
H	-1.81276800	-2.02384400	1.93589700
C	-1.90541200	0.55107900	2.80221200
H	-2.36798700	0.28118400	3.76108600
H	-0.87656400	0.17050300	2.80784000
H	-1.86283400	1.64315000	2.73519900
C	-3.50512100	-1.24985100	-1.57548300
H	-3.97727500	-1.42101500	-2.55343300
H	-2.78205100	-2.05632900	-1.40864800
H	-4.28886800	-1.32680000	-0.81602900
C	-1.83209800	0.21490200	-2.73817100
H	-2.37623200	0.16004600	-3.69046600
H	-1.26937900	1.15466200	-2.72075700
H	-1.11114800	-0.61241700	-2.72184200
C	-3.89332300	1.23444300	-1.76526200
H	-4.42657900	1.06769100	-2.71180100
H	-4.63370900	1.24444300	-0.96152100
H	-3.42597800	2.22377200	-1.80482300
C	3.03628000	-2.54781400	-0.13195400
H	3.93354100	-3.17670600	-0.06274200
H	2.35836900	-2.83416500	0.67771500
H	2.54201700	-2.76738200	-1.08373800
C	4.47872400	-0.79193800	-1.15996800
H	5.32356800	-1.48660800	-1.05980500
H	4.02460300	-0.94689700	-2.14357600
H	4.87782300	0.22262500	-1.12337500
C	4.10134000	-0.83461200	1.34961800
H	4.43932800	0.19606300	1.48464300
H	3.39664500	-1.07138400	2.15290100
H	4.97748700	-1.48820600	1.45870400
C	3.56139100	2.37369100	-0.30448400
H	4.33767800	1.91694700	0.31454800
H	3.78299400	2.17174900	-1.35653100
H	3.61951700	3.45985400	-0.15437400
C	1.13709200	2.67043200	-0.81597300
H	0.10519400	2.38869600	-0.59039500

H	1.24668800	3.74866600	-0.63606800
H	1.32833500	2.47809100	-1.87686700
C	1.86450000	2.22229700	1.55881400
H	1.99838000	3.29815900	1.73823400
H	0.83804600	1.95820800	1.82628900
H	2.54518100	1.67978400	2.22229200

(PTMS2)2Ge_1 E = -2323.37293331 a.u.

0 1

P	-1.63515800	0.47561300	0.21250300
P	1.88962700	-0.07697200	0.05231300
C	-4.83966100	0.25504800	1.53803000
H	-5.33333000	0.06911500	0.57863500
H	-5.49891900	-0.11620500	2.33256300
H	-4.73094800	1.33699900	1.66344700
C	-3.35725000	-2.47275300	1.28502700
H	-4.04195900	-2.92045100	2.01661500
H	-3.76450200	-2.64878700	0.28500800
H	-2.40038200	-3.00173700	1.35420200
C	-2.42384100	-0.38841400	3.38362400
H	-3.07729000	-0.84804500	4.13529900
H	-1.43408000	-0.85030800	3.46470400
H	-2.31794400	0.67429200	3.62392800
C	-3.69257300	-1.04286800	-2.31084300
H	-4.09304100	-0.96352400	-3.32958100
H	-3.05149800	-1.92958800	-2.26725800
H	-4.53660100	-1.19908600	-1.63121700
C	-1.35972700	0.79648400	-3.18218600
H	-1.81546700	1.00334900	-4.15851000
H	-0.71724100	1.64201100	-2.91818900
H	-0.72178200	-0.08780400	-3.28774400
C	-3.87360500	2.03977400	-1.85232600
H	-4.36360400	2.15926200	-2.82673800
H	-4.65063400	1.94225700	-1.08839500
H	-3.30623000	2.95126600	-1.63863900
C	3.40890200	-2.98796000	-0.76185100
H	4.31744400	-3.57707500	-0.93716100
H	2.84344500	-3.46650500	0.04359300
H	2.80003600	-3.02427500	-1.67040200
C	4.81517400	-0.39168900	-1.75443300
H	5.72439200	-0.96090200	-1.98455200
H	4.19063800	-0.36357100	-2.65266200
H	5.11124100	0.63420600	-1.51476500
C	4.93635900	-1.18152100	1.26571300
H	5.22494300	-0.16270400	1.54144700
H	4.38703300	-1.61819100	2.10538600
H	5.85384600	-1.76373900	1.11457500
C	3.80771700	2.67679700	0.75917800
H	4.36064000	2.09590100	1.50369000
H	4.30028100	2.56042800	-0.21108700
H	3.87379300	3.73449500	1.04371600
C	1.06088800	3.19558600	-0.61605800
H	0.01113700	2.88922200	-0.65019800
H	1.10670800	4.25995600	-0.35326700
H	1.49932800	3.06529100	-1.61027200
C	1.16716300	2.31574600	2.38615300
H	1.17338500	3.36140200	2.71826100
H	0.12947100	1.97371500	2.33135400
H	1.69482400	1.71187300	3.13073500
Si	-3.14677700	-0.61157400	1.63769700
Si	-2.71372200	0.53162000	-1.87028100
Si	3.87551100	-1.20112900	-0.31259300
Si	1.97713700	2.15682000	0.67917000
Ge	-0.01098500	-1.36524500	-0.21702500

(PTMS2)2Ge_4 E = -2323.37289640 a.u.

0 1

P	-1.63475000	0.43744700	0.30801900
P	1.89148300	-0.03334800	-0.06258000
C	3.83292900	2.54245800	1.10011300
H	4.28533100	2.65780100	0.11025900
H	3.91194900	3.50603200	1.61914300
H	4.41603400	1.81007000	1.66716100
C	1.05075100	3.29618400	-0.08459200
H	-0.00460600	3.01088800	-0.12576000
H	1.12565700	4.29899500	0.35434600
H	1.44613000	3.33355900	-1.10421300
C	1.23223500	1.88516700	2.70003700
H	0.19136800	1.56082500	2.60837500
H	1.77348400	1.15476800	3.30924300
H	1.25120100	2.85224400	3.21809800
C	4.96937700	-0.12922900	-1.63398200
H	5.29431800	0.79825500	-1.15322300
H	5.86536600	-0.69885000	-1.91028200
H	4.43256700	0.13195900	-2.55107600
C	4.76900900	-1.52968400	1.15068100
H	5.68000500	-2.11034200	0.95918100
H	5.05885300	-0.60912100	1.66679500
H	4.12828700	-2.10784400	1.82363000
C	3.37666200	-2.78846700	-1.33529100
H	2.71526300	-3.38887800	-0.70313700
H	2.86007900	-2.59919100	-2.28126800
H	4.27405300	-3.38174500	-1.54968200
C	-3.36059000	-2.66141900	0.79923400
H	-4.08748400	-3.22204000	1.40069300
H	-3.71617700	-2.64120700	-0.23485000
H	-2.41490100	-3.21406200	0.81604800
C	-2.42121700	-1.01935000	3.25596400
H	-3.07214600	-1.61616100	3.90660900
H	-1.43105400	-1.48748700	3.24385200
H	-2.31415600	-0.02314600	3.69705600
C	-4.83857100	-0.02970900	1.57244800
H	-5.51189700	-0.57046600	2.24919300
H	-4.73124100	0.99385600	1.94526100
H	-5.31642400	0.01396600	0.58822500
C	-3.88996700	2.33351400	-1.43614200
H	-4.39252900	2.61700400	-2.36931500
H	-4.65607500	2.09589500	-0.69218200
H	-3.32668800	3.19873400	-1.07244100
C	-1.38404300	1.36346400	-2.98916100
H	-0.75297400	2.16460300	-2.59258300
H	-0.73335100	0.52072300	-3.24555000
H	-1.85321800	1.72260400	-3.91367400
C	-3.70146700	-0.61558500	-2.43106600
H	-4.52692300	-0.89949300	-1.77029800
H	-4.12838000	-0.35489400	-3.40792100
H	-3.05649300	-1.49023000	-2.56607900
Si	-2.72131500	0.86126400	-1.73153900
Si	-3.14750900	-0.90247900	1.50083500
Si	1.99993400	2.04106700	0.97296500
Si	3.86436700	-1.16181100	-0.48192000
Ge	-0.00879900	-1.30330400	-0.41485900

(PPh2)2Ge_1 E = -1612.31103871 a.u.

0 1

P	-1.90293800	0.84022400	-0.42741500
P	1.81665100	-0.10520800	-1.45468700
Sn	-0.28163700	-1.29415700	-0.41213900
C	-1.60074400	0.56115500	1.41408100

C	-0.29158100	0.83945500	1.89271900
C	-2.57310800	0.12836400	2.34191000
C	0.02569100	0.67691100	3.25230400
H	0.45383400	1.26262000	1.22286200
C	-2.25092100	-0.02206600	3.69583500
H	-3.58361600	-0.07385100	2.00520600
C	-0.94966200	0.24312000	4.15784000
H	1.02751100	0.91120600	3.59774600
H	-3.01758200	-0.34216400	4.39435600
H	-0.70826700	0.12459800	5.20873300
C	-3.61124000	0.10433000	-0.69513600
C	-4.00088000	-1.21071800	-0.37128800
C	-4.55332600	0.94688600	-1.31892500
C	-5.29454300	-1.66855400	-0.65774400
H	-3.29477200	-1.88826800	0.10098200
C	-5.84803200	0.49073700	-1.61074900
H	-4.26972100	1.96343500	-1.57299500
C	-6.22270400	-0.81901000	-1.27989800
H	-5.57390400	-2.68549200	-0.40165700
H	-6.55764400	1.15580300	-2.09196700
H	-7.22260100	-1.17510100	-1.50535200
C	2.05877900	1.65989900	-0.90708100
C	3.14478500	2.06955100	-0.10841200
C	1.15014100	2.63610100	-1.36895700
C	3.31147400	3.42172000	0.22703700
H	3.86645900	1.33990500	0.24178900
C	1.31511100	3.98347600	-1.02367700
H	0.31231900	2.34414900	-1.99303600
C	2.39706800	4.38428400	-0.22446000
H	4.15781100	3.71933300	0.83826300
H	0.60065600	4.71722100	-1.38219100
H	2.52688100	5.42903700	0.03786900
C	3.23886800	-1.02928600	-0.66166900
C	3.32414200	-1.29279000	0.72057000
C	4.26030300	-1.51255600	-1.50304900
C	4.40111800	-2.02021700	1.24797700
H	2.54882800	-0.92732500	1.38769500
C	5.33962400	-2.24006600	-0.97798300
H	4.20685300	-1.31711300	-2.56901100
C	5.41189400	-2.49621400	0.39888800
H	4.44830900	-2.21665400	2.31423100
H	6.11712200	-2.60437800	-1.64145800
H	6.24415500	-3.06139400	0.80562000

(PPh2)2Ge_4 E = -1612.31046908 a.u.

0 1

P	-1.89070500	-0.12829800	0.06155800
P	1.82636700	0.58405200	0.64999100
Sn	0.25198000	-1.37238500	-0.32120500
C	2.34633000	1.37747500	-0.96995800
C	1.35350800	1.89937900	-1.82520800
C	3.69909500	1.59319400	-1.29963800
C	1.70373800	2.60290900	-2.98580300
H	0.30219000	1.76860100	-1.58149000
C	4.04754600	2.29572800	-2.46253200
H	4.48214400	1.22046800	-0.64796300
C	3.05340000	2.80119300	-3.31333800
H	0.92354700	2.99587900	-3.62999300
H	5.09567300	2.45203400	-2.69791000
H	3.32533500	3.34410800	-4.21249600
C	3.25464700	-0.57565300	1.03784600
C	3.91216700	-1.37937600	0.08366600
C	3.65247800	-0.67160400	2.38588100
C	4.94246400	-2.24910600	0.46699400
H	3.62831900	-1.31764500	-0.96319300

C	4.67714800	-1.54881800	2.77333300
H	3.16289700	-0.05065200	3.12981800
C	5.32644800	-2.33921400	1.81443800
H	5.43911600	-2.85775300	-0.28187700
H	4.97005100	-1.60783000	3.81662700
H	6.12171500	-3.01516700	2.11118600
C	-2.35246500	1.42503100	0.94086800
C	-3.56464200	2.08347600	0.64824600
C	-1.47278000	1.98982100	1.88516600
C	-3.89515600	3.27713900	1.30366300
H	-4.24454800	1.66972300	-0.08895600
C	-1.80431500	3.18988900	2.52762400
H	-0.53087200	1.50194300	2.11057200
C	-3.01732100	3.83592600	2.24500900
H	-4.83237400	3.77236700	1.07140800
H	-1.11511100	3.61562900	3.24922900
H	-3.27345000	4.76255600	2.74775700
C	-3.43818100	-1.02750500	-0.38648000
C	-4.50320800	-1.15387500	0.52954400
C	-3.54155300	-1.65453000	-1.64392700
C	-5.64563200	-1.88987900	0.19038900
H	-4.43389500	-0.68619600	1.50609500
C	-4.67955600	-2.40546400	-1.97363200
H	-2.74172800	-1.54272900	-2.36904800
C	-5.73627500	-2.52314400	-1.05969900
H	-6.45732600	-1.97836700	0.90503500
H	-4.74306300	-2.88446500	-2.94508500
H	-6.61981200	-3.09754300	-1.31740600

(PH2)2Sn_1 E = -688.43826420 a.u.

0 1

P	-1.86521700	1.07520200	-0.11643800
H	-2.84566100	0.55728100	0.79446900
H	-1.36643400	2.12157900	0.72960100
P	1.86516400	1.07523500	0.11643400
H	2.84571100	0.55739000	-0.79439800
H	1.36644000	2.12166800	-0.72956100
Sn	0.00001500	-0.75229000	-0.00000100

(PH2)2Sn_2 E = -688.43746508 a.u.

0 1

P	-1.87259600	1.07768800	-0.11750000
H	-2.91587200	0.43091700	0.62775900
H	-1.50010100	2.02732300	0.89270800
P	1.87260300	1.07777000	-0.11751300
H	1.49831500	2.02784900	0.89151900
H	2.91527500	0.43171800	0.62917100
Sn	0.00004500	-0.74499400	0.00968100

(PMe2)2Sn_2 E = -845.66163199 a.u.

0 1

P	-1.72539200	0.89230100	-0.46436900
P	1.88460000	0.39184700	-0.41070100
C	-3.39160100	-0.02771300	-0.46628800
H	-4.19836400	0.70515600	-0.56451400
H	-3.43319900	-0.69472900	-1.33167000
H	-3.56159000	-0.61528200	0.44107300
C	1.78330200	2.26566400	-0.36076700
H	2.57874000	2.69172500	-0.97871500
H	0.81801400	2.57269200	-0.77023300
H	1.88056900	2.64437400	0.66041800
Sn	-0.05905100	-1.11220500	0.09301700

C	-1.85072500	1.73324200	1.24424900
H	-0.88708300	2.18239200	1.49795600
H	-2.59647700	2.53226300	1.18370400
H	-2.14171000	1.04546200	2.04388700
C	3.54021200	-0.02974400	0.37112500
H	3.63580300	-1.11533800	0.44760100
H	4.35356500	0.34673800	-0.25515400
H	3.62904700	0.40387700	1.37096400

(PMe2)2Sn_4 E = -845.66127323 a.u.

0 1

P	1.81363100	0.69497100	0.47434500
P	-1.81360200	0.69506600	-0.47437600
C	3.46621500	-0.15046300	0.08601600
H	4.28375800	0.52307700	0.35873000
H	3.55924700	-1.05904100	0.68677600
H	3.56180100	-0.41420300	-0.97084900
C	-1.77413300	2.03736400	0.86721100
H	-2.07306000	1.63924600	1.84046200
H	-0.76613500	2.44732800	0.95644400
H	-2.45831700	2.84279300	0.58532900
Sn	-0.00001700	-1.10902300	0.00000900
C	1.77410400	2.03736100	-0.86714600
H	0.76604900	2.44716000	-0.95648800
H	2.45812200	2.84288800	-0.58513800
H	2.07322100	1.63933700	-1.84038000
C	-3.46613900	-0.15051800	-0.08608000
H	-4.28374400	0.52294700	-0.35879700
H	-3.55906800	-1.05909700	-0.68685600
H	-3.56171700	-0.41428500	0.97078000

(PtBu2)2Sn_2 E = -1317.22326296 a.u.

0 1

P	2.01196500	-0.21926200	0.28898100
P	-1.88633700	-0.63283400	-0.28299600
C	3.64061500	0.83827000	0.25899500
C	-2.96142900	0.49041100	-1.47574800
Sn	-0.04652300	1.22860700	0.35710200
C	2.17923000	-1.91778200	-0.64243400
C	-2.81140800	-0.86955200	1.42874700
C	-3.99156700	-0.41877300	-2.17906000
H	-4.71630900	-0.83688400	-1.47617200
H	-4.54702600	0.15866400	-2.93181100
H	-3.49474800	-1.25351900	-2.68375300
C	-1.97641400	1.00537100	-2.54686900
H	-1.28863200	1.76346300	-2.14325900
H	-1.37971400	0.18886100	-2.96856000
H	-2.53100800	1.48108300	-3.36642400
C	-3.67693100	1.68884000	-0.83260200
H	-4.17612500	2.28273400	-1.61156500
H	-4.44549000	1.37201500	-0.12123700
H	-2.97697400	2.34952500	-0.30765500
C	-4.22008900	-1.44319100	1.18119800
H	-4.65723100	-1.76320800	2.13726200
H	-4.89341900	-0.69944200	0.74420700
H	-4.18700900	-2.31209300	0.51562400
C	-1.97276900	-1.93411000	2.16879500
H	-1.92705700	-2.86896400	1.60094300
H	-0.94463000	-1.59446300	2.34209400
H	-2.42604200	-2.14601100	3.14656400
C	-2.91714300	0.37824900	2.32471300
H	-3.43348100	1.20607800	1.83395400
H	-3.47376700	0.12917100	3.23974300
H	-1.92701400	0.73550800	2.63521400

C	1.11718900	-2.85765000	-0.03827400
H	1.28925300	-3.01366900	1.03166000
H	0.10574500	-2.46578800	-0.17791000
H	1.17520400	-3.83198800	-0.54248800
C	1.90418000	-1.73226900	-2.14860100
H	2.61365700	-1.03999600	-2.61113800
H	1.99045300	-2.70150500	-2.66005000
H	0.89224600	-1.35013500	-2.31232400
C	3.56450300	-2.55660300	-0.43183300
H	3.56416800	-3.54608600	-0.90793600
H	4.37279100	-1.97632400	-0.88456000
H	3.78381900	-2.69681700	0.63097300
C	4.21051800	0.97152900	-1.16629400
H	5.10480000	1.60954700	-1.14373400
H	4.50491000	0.00678000	-1.58751000
H	3.47989400	1.42993000	-1.84026400
C	4.69117500	0.22435400	1.20904300
H	5.01307100	-0.76751100	0.88856900
H	5.57791700	0.87229400	1.23680900
H	4.29538800	0.14175700	2.22604100
C	3.29355800	2.24477000	0.78483400
H	2.63200700	2.78571000	0.10073300
H	2.81322300	2.20543500	1.76872000
H	4.21955800	2.82576300	0.88670500

(PtBu2)2Sn_4 E = -1317.22326296 a.u.

0 1

P	-1.87638400	0.67370800	0.05992200
P	2.01686200	0.13274500	-0.33574100
C	-2.98973500	0.30821900	-1.50717500
C	2.16904500	2.03047300	0.05128100
C	-2.77319700	0.06197700	1.69120100
C	3.64437700	-0.86345200	0.02053700
C	-4.14664000	0.74980700	1.80935400
H	-4.86536600	0.35122300	1.08688300
H	-4.55817200	0.57927000	2.81394800
H	-4.06459900	1.83061800	1.65411100
C	-2.94739900	-1.45941100	1.85480200
H	-3.47440900	-1.67179600	2.79613200
H	-3.52387500	-1.90464900	1.04135300
H	-1.98080800	-1.97812000	1.90503800
C	-1.86680800	0.57945200	2.82924000
H	-2.30464200	0.31738600	3.80178800
H	-0.86386100	0.13596300	2.78392400
H	-1.75633500	1.66768800	2.78230100
C	-3.74650100	-1.02910100	-1.51498400
H	-4.25390000	-1.15915500	-2.48159500
H	-3.07092900	-1.88080800	-1.37527200
H	-4.51388500	-1.06741500	-0.73604000
C	-2.02635100	0.34911400	-2.71278900
H	-2.60275100	0.35924900	-3.64740700
H	-1.39365400	1.24337500	-2.69437900
H	-1.37150900	-0.53260500	-2.74381700
C	-3.98956200	1.47540500	-1.65762500
H	-4.57012800	1.35115000	-2.58271300
H	-4.69423000	1.52200200	-0.82337900
H	-3.46452900	2.43470700	-1.70747600
C	3.30264700	-2.36431100	-0.06244900
H	4.22847000	-2.94552500	0.03962900
H	2.62216000	-2.67280600	0.73764500
H	2.84632500	-2.62748500	-1.02287600
C	4.71097000	-0.56087200	-1.05390600
H	5.59473300	-1.18815600	-0.87384000
H	4.33020800	-0.78622800	-2.05489800
H	5.03426800	0.48115200	-1.03978900

CXX

C	4.19181000	-0.56184400	1.42934700
H	4.48384200	0.48482500	1.54656500
H	3.44983100	-0.79762600	2.19884200
H	5.08333200	-1.17743000	1.61239200
C	3.56088500	2.58028200	-0.30992100
H	4.35650900	2.16272800	0.31238600
H	3.80269500	2.39756300	-1.36129700
H	3.55590700	3.66689800	-0.15147100
C	1.12507700	2.74115700	-0.83380900
H	0.10988800	2.39768200	-0.61557400
H	1.16744900	3.82129200	-0.63785800
H	1.33198500	2.57619300	-1.89643100
C	1.85745500	2.29689000	1.53696900
H	1.92570200	3.37487800	1.74033100
H	0.84463400	1.96631500	1.78243800
H	2.55925900	1.78038100	2.19849300
Sn	-0.05126400	-1.29224500	-0.19342500

(PTMS2)2Sn_2 E = -2322.95910479 a.u.

0 1

P	-1.72036300	0.40391300	0.38091300
P	1.97415400	0.17630900	-0.30498200
C	-4.97382600	0.16173700	1.52389700
H	-5.41531400	0.41941500	0.55559300
H	-5.73084300	-0.37936800	2.10500700
H	-4.74117000	1.09327700	2.04962800
C	-3.82621200	-2.50304200	0.37704900
H	-4.57869500	-3.08396300	0.92567100
H	-4.22286300	-2.28850100	-0.61964900
H	-2.93971600	-3.13554000	0.25553400
C	-2.74848200	-1.37594700	3.05218800
H	-3.50465900	-1.93459400	3.61724000
H	-1.85193300	-2.00184500	2.97955100
H	-2.48561500	-0.47941600	3.62258500
C	-3.83886600	0.05520600	-2.47494900
H	-4.22850100	0.51660700	-3.39132000
H	-3.34659500	-0.88312500	-2.75024700
H	-4.69126900	-0.18332000	-1.83096600
C	-1.18772700	1.62643800	-2.80215100
H	-1.54513700	2.24710300	-3.63340500
H	-0.38258200	2.16365900	-2.29292400
H	-0.75761500	0.71184500	-3.22445800
C	-3.52196300	2.85286500	-1.14749200
H	-3.97753000	3.31287300	-2.03325300
H	-4.31005200	2.66745700	-0.41112900
H	-2.81825200	3.56856000	-0.71072900
C	3.71833500	-2.47472500	-1.49391700
H	4.66253300	-3.01551300	-1.63291300
H	3.00620200	-3.15623700	-1.01735700
H	3.32891200	-2.21274500	-2.48282900
C	5.27395900	0.20925700	-1.30681000
H	6.21635900	-0.32967700	-1.46536300
H	4.89552200	0.53328400	-2.28116400
H	5.48962600	1.10221100	-0.71297400
C	4.63768200	-1.41049000	1.28609300
H	4.76648300	-0.53513200	1.93091900
H	3.92858200	-2.08642900	1.77460100
H	5.60569300	-1.92183700	1.21254100
C	3.75634000	2.67944900	1.22042700
H	4.45668700	1.93600300	1.61397800
H	4.10780800	3.00000800	0.23490300
H	3.78175300	3.54926400	1.88893800
C	0.83178300	3.33677700	0.40429300
H	-0.19594500	2.96155000	0.38164200
H	0.86066700	4.23942000	1.02754100

H	1.13367000	3.60919100	-0.61170900
C	1.38217900	1.46920100	2.84594900
H	1.37922300	2.32081100	3.53800100
H	0.36228500	1.07797600	2.77620800
H	2.02830500	0.68880800	3.26057100
Sn	0.03055700	-1.41119300	-0.40521900
Si	-3.40836300	-0.90495700	1.32918200
Si	-2.62277100	1.24271300	-1.61440900
Si	4.00938000	-0.91706800	-0.44196200
Si	1.97604500	2.00816100	1.12477800

(PTMS2)2Sn_4 E = -2322.95909777 a.u.

0 1

P	-1.71152800	0.54626500	0.20577000
P	2.00381600	0.04099000	-0.02259500
C	3.78717500	2.90116200	0.63028200
H	4.25062500	2.83978500	-0.35913500
H	3.80130400	3.95287700	0.94308800
H	4.39930700	2.33441900	1.33856800
C	0.99157400	3.25545900	-0.69184100
H	-0.04505400	2.90505800	-0.69149500
H	0.99920800	4.32478100	-0.44571700
H	1.40816700	3.12802900	-1.69579500
C	1.20239300	2.41658200	2.31263200
H	0.17773200	2.03430000	2.27821000
H	1.76617100	1.83880300	3.05147500
H	1.17244500	3.46393300	2.63825000
C	5.08394700	-0.15541700	-1.57629500
H	5.32901000	0.87687000	-1.30930000
H	6.02488400	-0.69702000	-1.73440200
H	4.53251900	-0.14044900	-2.52139200
C	4.98209100	-0.95715500	1.44204700
H	5.93093800	-1.50233500	1.36344500
H	5.20633600	0.06871500	1.74975600
H	4.38180000	-1.42300900	2.22957000
C	3.70226900	-2.80364800	-0.70960400
H	3.10747800	-3.31717600	0.05242700
H	3.15993500	-2.85763600	-1.65876700
H	4.64659400	-3.34945900	-0.82660300
C	-3.55936000	-2.27740600	1.40182500
H	-4.28937500	-2.65476400	2.12930600
H	-3.94718000	-2.47258800	0.39759500
H	-2.63721800	-2.85673600	1.52431800
C	-2.51039000	-0.16195700	3.41409900
H	-3.18561900	-0.55181600	4.18568700
H	-1.54727700	-0.67374100	3.51530300
H	-2.34489300	0.90258200	3.60791400
C	-4.90380700	0.52555000	1.55803200
H	-5.58272100	0.20205700	2.35682000
H	-4.74309400	1.60324900	1.66224400
H	-5.40218000	0.34531400	0.60003600
C	-3.84984100	2.19381400	-1.89429600
H	-4.35279000	2.30811100	-2.86267800
H	-4.61291300	2.18918600	-1.10998500
H	-3.20986400	3.06707200	-1.73302000
C	-1.46689200	0.69459000	-3.20738000
H	-0.73049100	1.46908900	-2.97197700
H	-0.93229500	-0.25626000	-3.31424800
H	-1.91907800	0.93498200	-4.17763900
C	-3.93156900	-0.90265400	-2.21859000
H	-4.76147800	-0.96495200	-1.50692000
H	-4.36012000	-0.82092900	-3.22573600
H	-3.36702600	-1.83963800	-2.16630400
Si	-2.81227400	0.59944300	-1.86238000
Si	-3.25305500	-0.41632000	1.68059900

Si	1.98777900	2.27672400	0.59164500
Si	4.05500700	-1.00046900	-0.21865900
Sn	0.00883900	-1.44048700	-0.19005700

(PPh2)2Sn_2 E = -1612.31103871 a.u.

0 1

P	-1.90293800	0.84022400	-0.42741500
P	1.81665100	-0.10520800	-1.45468700
Sn	-0.28163700	-1.29415700	-0.41213900
C	-1.60074400	0.56115500	1.41408100
C	-0.29158100	0.83945500	1.89271900
C	-2.57310800	0.12836400	2.34191000
C	0.02569100	0.67691100	3.25230400
H	0.45383400	1.26262000	1.22286200
C	-2.25092100	-0.02206600	3.69583500
H	-3.58361600	-0.07385100	2.00520600
C	-0.94966200	0.24312000	4.15784000
H	1.02751100	0.91120600	3.59774600
H	-3.01758200	-0.34216400	4.39435600
H	-0.70826700	0.12459800	5.20873300
C	-3.61124000	0.10433000	-0.69513600
C	-4.00088000	-1.21071800	-0.37128800
C	-4.55332600	0.94688600	-1.31892500
C	-5.29454300	-1.66855400	-0.65774400
H	-3.29477200	-1.88826800	0.10098200
C	-5.84803200	0.49073700	-1.61074900
H	-4.26972100	1.96343500	-1.57299500
C	-6.22270400	-0.81901000	-1.27989800
H	-5.57390400	-2.68549200	-0.40165700
H	-6.55764400	1.15580300	-2.09196700
H	-7.22260100	-1.17510100	-1.50535200
C	2.05877900	1.65989900	-0.90708100
C	3.14478500	2.06955100	-0.10841200
C	1.15014100	2.63610100	-1.36895700
C	3.31147400	3.42172000	0.22703700
H	3.86645900	1.33990500	0.24178900
C	1.31511100	3.98347600	-1.02367700
H	0.31231900	2.34414900	-1.99303600
C	2.39706800	4.38428400	-0.22446000
H	4.15781100	3.71933300	0.83826300
H	0.60065600	4.71722100	-1.38219100
H	2.52688100	5.42903700	0.03786900
C	3.23886800	-1.02928600	-0.66166900
C	3.32414200	-1.29279000	0.72057000
C	4.26030300	-1.51255600	-1.50304900
C	4.40111800	-2.02021700	1.24797700
H	2.54882800	-0.92732500	1.38769500
C	5.33962400	-2.24006600	-0.97798300
H	4.20685300	-1.31711300	-2.56901100
C	5.41189400	-2.49621400	0.39888800
H	4.44830900	-2.21665400	2.31423100
H	6.11712200	-2.60437800	-1.64145800
H	6.24415500	-3.06139400	0.80562000

(PPh2)2Sn_2 E = Ôªø0Ôªø0Ôªø-1612.31046908 a.u.

0 1

P	-1.89070500	-0.12829800	0.06155800
P	1.82636700	0.58405200	0.64999100
Sn	0.25198000	-1.37238500	-0.32120500
C	2.34633000	1.37747500	-0.96995800
C	1.35350800	1.89937900	-1.82520800
C	3.69909500	1.59319400	-1.29963800
C	1.70373800	2.60290900	-2.98580300
H	0.30219000	1.76860100	-1.58149000

C	4.04754600	2.29572800	-2.46253200
H	4.48214400	1.22046800	-0.64796300
C	3.05340000	2.80119300	-3.31333800
H	0.92354700	2.99587900	-3.62999300
H	5.09567300	2.45203400	-2.69791000
H	3.32533500	3.34410800	-4.21249600
C	3.25464700	-0.57565300	1.03784600
C	3.91216700	-1.37937600	0.08366600
C	3.65247800	-0.67160400	2.38588100
C	4.94246400	-2.24910600	0.46699400
H	3.62831900	-1.31764500	-0.96319300
C	4.67714800	-1.54881800	2.77333300
H	3.16289700	-0.05065200	3.12981800
C	5.32644800	-2.33921400	1.81443800
H	5.43911600	-2.85775300	-0.28187700
H	4.97005100	-1.60783000	3.81662700
H	6.12171500	-3.01516700	2.11118600
C	-2.35246500	1.42503100	0.94086800
C	-3.56464200	2.08347600	0.64824600
C	-1.47278000	1.98982100	1.88516600
C	-3.89515600	3.27713900	1.30366300
H	-4.24454800	1.66972300	-0.08895600
C	-1.80431500	3.18988900	2.52762400
H	-0.53087200	1.50194300	2.11057200
C	-3.01732100	3.83592600	2.24500900
H	-4.83237400	3.77236700	1.07140800
H	-1.11511100	3.61562900	3.24922900
H	-3.27345000	4.76255600	2.74775700
C	-3.43818100	-1.02750500	-0.38648000
C	-4.50320800	-1.15387500	0.52954400
C	-3.54155300	-1.65453000	-1.64392700
C	-5.64563200	-1.88987900	0.19038900
H	-4.43389500	-0.68619600	1.50609500
C	-4.67955600	-2.40546400	-1.97363200
H	-2.74172800	-1.54272900	-2.36904800
C	-5.73627500	-2.52314400	-1.05969900
H	-6.45732600	-1.97836700	0.90503500
H	-4.74306300	-2.88446500	-2.94508500
H	-6.61981200	-3.09754300	-1.31740600

GeCubane E = -7449.31092278 a.u.

0 1

Ge	-1.23152000	1.18236700	1.65941700
Ge	-1.10989900	0.28264000	-2.08716500
Si	2.05591800	-0.42623100	3.84946100
Si	1.23039800	1.17627700	5.44023300
Si	1.62876100	-2.64329200	4.66750100
P	-1.91625500	-0.74886500	0.12139800
Si	4.40536900	-0.10651600	3.47833200
P	0.95303100	-0.15423000	1.81018900
Si	2.26157000	-2.12931500	-3.09776500
Si	4.21917000	-0.87711600	-3.70715600
C	2.42140700	1.25586500	6.93079000
H	3.38708300	1.68356100	6.64224100
H	2.60157800	0.26719200	7.36360900
H	1.99289100	1.89515600	7.71314200
C	-0.50097400	0.67902400	6.06310000
H	-0.87313500	1.43316300	6.76753600
H	-0.48222400	-0.28538700	6.57915800
H	-1.21365300	0.60945100	5.23505900
C	1.12065300	2.90963800	4.66507200
H	0.41384800	2.91789900	3.82869100
H	2.09355100	3.24308200	4.29288100
H	0.77148600	3.63539800	5.41010700
C	-0.22710900	-3.05373000	4.52729700

H	-0.83742000	-2.38080500	5.13831800
H	-0.41228500	-4.08246900	4.86150000
H	-0.56722600	-2.96821100	3.49098500
C	2.13940300	-2.75528200	6.50758700
H	3.18778100	-2.47778700	6.65644800
H	2.00917600	-3.78514900	6.86289000
H	1.52159600	-2.10484800	7.13803900
C	2.62358500	-3.94536900	3.68990000
H	2.36309800	-3.93003900	2.62646800
H	2.40249700	-4.94859000	4.07558700
H	3.70180300	-3.78021500	3.77785400
C	5.38989500	-0.70544000	5.00353400
H	5.07933800	-0.18970300	5.91818400
H	6.45961600	-0.51297700	4.85398900
H	5.26300000	-1.78291300	5.16061200
C	4.79077400	1.73797200	3.18336100
H	4.22792000	2.12524300	2.32791200
H	5.85932500	1.87067700	2.97145100
H	4.54317300	2.34614200	4.06004700
C	4.96829200	-1.10427100	1.95732200
H	4.79884600	-2.17649400	2.09385900
H	6.03811000	-0.94487500	1.77206600
H	4.42025600	-0.78719700	1.06344400
C	3.78359800	0.95273200	-4.00714000
H	3.01749500	1.06181200	-4.77871000
H	4.67582300	1.50402400	-4.32948500
H	3.41055100	1.42290700	-3.09107200
C	5.53874200	-0.98143900	-2.33300100
H	5.14864900	-0.61148900	-1.37911600
H	6.40910200	-0.36993800	-2.60218200
H	5.88352300	-2.01025200	-2.18387900
C	4.95480300	-1.59438700	-5.31911400
H	5.17088500	-2.66363400	-5.23260000
H	5.89388100	-1.07943800	-5.55841400
H	4.27284100	-1.45067300	-6.16371800
Si	0.83875600	-2.44603100	-5.00924500
C	-0.87781000	-3.06078300	-4.45669400
H	-0.81007600	-4.00766300	-3.91237600
H	-1.52698600	-3.21226100	-5.32792700
H	-1.36119400	-2.33069500	-3.79989800
C	0.63532300	-0.81096400	-5.96842900
H	0.20452900	-0.03321000	-5.33054400
H	-0.03706000	-0.95691600	-6.82275500
H	1.59473900	-0.44654800	-6.35274300
C	1.60662000	-3.75578400	-6.17164200
H	2.62005500	-3.48444300	-6.48514400
H	0.99057900	-3.85654600	-7.07400600
H	1.65289700	-4.73742100	-5.68701100
Si	2.93057000	-4.24667800	-2.18776500
C	3.67102600	-4.02109500	-0.45000000
H	4.54236600	-3.36006700	-0.46997500
H	3.98359300	-4.99116100	-0.04394500
H	2.93531800	-3.58977000	0.23551900
C	1.45736000	-5.45394600	-2.08397600
H	0.67651200	-5.06885600	-1.42028600
H	1.79368500	-6.41932500	-1.68554500
H	1.01214000	-5.63274600	-3.06735000
C	4.26401400	-5.02159400	-3.31998000
H	3.91672300	-5.11377300	-4.35422500
H	4.51830000	-6.02595800	-2.95915800
H	5.18350700	-4.42544500	-3.31859400
Ge	0.13925600	-2.22281100	0.54076700
Si	-4.04021200	-1.70125700	0.29553100
Si	-3.83267100	-4.09229700	0.19643500
Si	-4.99991300	-1.02743400	2.39224300
P	1.05951500	-0.95012500	-1.47743600

Si	-5.41151300	-0.94309800	-1.52331200
C	-3.12346600	-4.79470900	1.82238700
H	-3.77429600	-4.57367200	2.67505800
H	-2.13175600	-4.38212800	2.03211200
H	-3.02631700	-5.88505600	1.74668100
C	-2.68887700	-4.59391600	-1.24267500
H	-2.59328500	-5.68596200	-1.29118200
H	-1.68660200	-4.17325000	-1.10738100
H	-3.07265700	-4.24171600	-2.20301500
C	-5.55451300	-4.87042200	-0.09765500
H	-5.97170500	-4.56985400	-1.06568300
H	-6.26742700	-4.58722300	0.68219900
H	-5.47027000	-5.96468900	-0.09693200
C	-3.74588100	-1.26116100	3.80586400
H	-3.40882400	-2.29941400	3.88273100
H	-4.20057500	-0.97642800	4.76323000
H	-2.86384400	-0.62913000	3.65014900
C	-6.54006100	-2.09867200	2.75471200
H	-7.27599800	-2.04291800	1.94512000
H	-7.02403300	-1.75362900	3.67703100
H	-6.26673400	-3.15063700	2.89218200
C	-5.53070900	0.80541700	2.33489200
H	-4.67464300	1.46109400	2.14733800
H	-5.97310600	1.09742600	3.29536800
H	-6.27617700	0.98486200	1.55273600
C	-7.24292400	-1.33218300	-1.14147400
H	-7.39790400	-2.39593200	-0.93181300
H	-7.86424000	-1.06290700	-2.00482600
H	-7.60229100	-0.76121400	-0.27947800
C	-4.93268500	-1.81809800	-3.14867700
H	-3.88462300	-1.63208300	-3.40312100
H	-5.55256000	-1.43995100	-3.97122400
H	-5.08345700	-2.90108200	-3.08420900
C	-5.23097500	0.93742400	-1.77244800
H	-5.49536900	1.49278000	-0.86817600
H	-5.88598600	1.27315500	-2.58591000
H	-4.20243800	1.19861700	-2.04094500
Ge	2.16106000	0.96148900	-0.16195200
Si	-0.27388200	4.29572800	-1.05164800
Si	-2.58001200	4.82044300	-1.44165300
Si	0.59968500	5.56983900	0.78571300
P	-0.13975800	2.03735800	-0.49560600
Si	1.01412000	4.64574600	-3.04505600
C	-3.65070500	4.07953900	-0.05027200
H	-3.38834000	4.51461100	0.91943000
H	-3.51413600	2.99531900	0.01840800
H	-4.71322900	4.27504500	-0.23783000
C	-3.12885400	4.12207300	-3.12812800
H	-4.20950500	4.25162800	-3.26195800
H	-2.90203200	3.05373600	-3.21048600
H	-2.61883900	4.63996200	-3.94910900
C	-2.82061600	6.71661000	-1.45643500
H	-2.17591100	7.19926300	-2.19683000
H	-2.59990100	7.15750900	-0.47762600
H	-3.86148900	6.95938600	-1.70424300
C	-0.65556600	5.60649900	2.22083400
H	-1.54829700	6.18012800	1.94803900
H	-0.20781400	6.07963400	3.10355300
H	-0.97189900	4.59736600	2.50174500
C	0.93407300	7.36575300	0.22909400
H	1.72172200	7.40996600	-0.52996900
H	1.26208800	7.96577400	1.08745800
H	0.03552200	7.83330900	-0.18545100
C	2.23593700	4.79609300	1.38209100
H	2.08490000	3.76077200	1.70538100
H	2.64038400	5.35971100	2.23163700

H	2.98639200	4.79279200	0.58557200
C	0.57412300	6.34516200	-3.80179300
H	-0.47459000	6.38289300	-4.11290800
H	1.19514700	6.53291600	-4.68670000
H	0.74607300	7.15982000	-3.09090200
C	0.60898200	3.28425800	-4.31475700
H	0.85054200	2.29465800	-3.91622500
H	1.19153400	3.43143500	-5.23235300
H	-0.45298200	3.29242000	-4.57819100
C	2.87785300	4.63052900	-2.63834000
H	3.15052600	5.50023500	-2.03056600
H	3.47237100	4.66205500	-3.55980400
H	3.15975500	3.72797700	-2.08450800