CONFORMATIONAL DEPENDENCE OF σ-ELECTRON DELOCALIZATION IN THE CATENAE X_nMe_{2n+2}, X = Si, Ge, Sn, AND Pb

by

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Thesis directed by Professor Josef Michl

Abstract

Bonds of σ type are the most common chemical bonds, dominating bonding in all molecules and defining the framework of a molecule. It has been long known that electrons in σ bonds can delocalize throughout a molecule. However, the nature of σ-electron delocalization is not fully understood due to its complexity. One of the important aspects of σ-electron delocalization is its conformational dependence, first noted in oligosilanes where properties of a molecule change drastically when it changes conformation. This dissertation describes efforts to understand the conformational dependence of σ delocalization in oligosilanes and their heavier analogs using simple intuitive models and density functional theory (DFT) calculations. The first part of the dissertation focuses on studying the conformational dependence of electron delocalization in oligosilanes. It is shown that oligosilanes can exist as two distinct chromophores, σ-delocalized conformers with large dihedral angles and σ-localized conformers with small dihedral angles. Properties of a conformer are dictated by the shape of frontier molecular orbitals, which is different for conformers with small and large dihedral angles. The origin of the conformational dependence is found in the interplay between two delocalization mechanisms, which can lead to enhancement of delocalization or to its complete annihilation. The second part of the dissertation describes characteristics of σ-electron delocalization in linear infinite polysilane, polygermane, polystannane, and polyplumbane. The conformational dependence of electron delocalization is confirmed in all these molecules. Effective hole mass is used to indicate an extent of the delocalization, while a position of the Fermi level in

reciprocal space is used to determine the dominant mechanism of delocalization. The simple model used to explain the origin of the conformational dependence of electron delocalization in saturated compounds is verified by comparison with density functional theory calculations. Relatively simple analysis presented here provides an important insight into properties of a complex ubiquitous phenomenon of delocalization of electrons through σ bonds.

To my mother, Sofija, and the memory of my father.

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Vincent van Gogh

Chapter I

Introduction

1.1. Motivation

While π-electron delocalization has been studied even before quantum mechanics was used in chemistry[1] and its origins and effects are now a part of classical chemical education, ubiquitous σ-electron delocalization is far from fully understood in simple, intuitive terms. It is harder to study both experimentally and theoretically. Molecules composed of only σ-bonds are harder to study photo-physically as they usually do not possess chromophores and do not absorb in the near-UV/VIS region. Unlike rigid π-molecules, many σ-bonded molecules can explore whole conformational space which creates additional complications for techniques like nuclear magnetic resonance (NMR). Theoretically, the description of σ delocalization requires at least two orbitals per non-hydrogen atom, which makes it more complex than π delocalization. Over last decades, experimental studies of σ delocalization in oligo- and polysilanes have become possible, and much has been learned about its effects and conformational dependence.[2,3] Intuitive explanations have been proposed, but none of them offered a full explanation of the noted strong conformational dependence of σ delocalization.[4,5,6]

This thesis aims to explain the origin of the conformational dependence in terms of simple models. Oligosilanes are the starting point of the study because they have been extensively investigated experimentally. The work extends naturally to polysilanes, in which we study how effects of the delocalization combine with complex helical symmetry, resulting in phenomena like conformation-dependent conductivity.[7] Finally, we study germanes, stannanes, and plumbanes in order to see if the similarities and differences between electron behavior in catenanes of various

elements of group 14 can be explained in terms of simple models. Alkanes are not a part of the study because of additional complexities that arise due to similar electronegativity of carbon and hydrogen: the influence of lateral substituents on electron delocalization cannot be disregarded in alkanes and a correct description of the delocalization requires more complex models. Similarly, when available, spectroscopic data on alkanes are hard to interpret due to close transition energies.

1.2. Methods

Regardless of their complexity, commonly used electronic structure methods are based on non-relativistic time-independent Schrödinger equation:[8]

$$\hat{H}\Psi(\boldsymbol{r},\boldsymbol{R}) = E\Psi(\boldsymbol{r},\boldsymbol{R}) \tag{1}$$

where $\Psi(\boldsymbol{r},\boldsymbol{R})$ is the total wave function describing a system with the Hamiltonian $\hat{H}$ and energy E. The total wave function depends on the electron coordinates, $\boldsymbol{r}$, and the nuclear coordinates, $\boldsymbol{R}$. Full, non-relativistic Hamiltonian is:

$$\hat{H} = T_{nuc}(\boldsymbol{R}) + T_{el}(\boldsymbol{r}) + V_{nuc}(\boldsymbol{R_1},\boldsymbol{R_2}) + V_{el}(\boldsymbol{r_1},\boldsymbol{r_2}) + V_{nuc\text{-}el}(\boldsymbol{r},\boldsymbol{R}) \tag{2}$$

where $T_{nuc}(\boldsymbol{R})$ and $T_{el}(\boldsymbol{r})$ are nuclear and electron kinetic energy operators, respectively, and $V_{nuc}(\boldsymbol{R_1},\boldsymbol{R_2})$, $V_{el}(\boldsymbol{r_1},\boldsymbol{r_2})$, and $V_{nuc\text{-}el}(\mathbf{r},\boldsymbol{R})$ represent nuclear-nuclear, electron-electron, and nuclear-electron potential energy operators, respectively.

Electronic structure methods differ in the approximations they2 make in order to solve equation 1. The first approximation made in most methods is the Born-Oppenheimer approximation which separates nuclear, $\psi_{nuc}(\boldsymbol{R})$, and electron, $\psi_{el}(\boldsymbol{r})$, motion:

$$\Psi(\boldsymbol{r},\boldsymbol{R}) = \psi_{el}(\boldsymbol{r})\psi_{nuc}(\boldsymbol{R}) \tag{3}$$

and proceeds to freeze nuclear positions.[9] This approximation is rooted in the large mass difference

between electrons and nuclei, which allows us to separate time scales for their motion and assume that electrons instantaneously adapt to a given configuration of nuclei. The time-independent Schrödinger equation is then solved for the electrons moving in the potential of the stationary nuclei, and the energy depends only parametrically on the nuclear positions.

The Born-Oppenheimer approximation leads to electronic Schrödinger equation:

$$\hat{H}_{el}(\boldsymbol{r};\mathbf{R})\psi_{el}(\boldsymbol{r};\mathbf{R}) = E_{el}(\boldsymbol{r};\mathbf{R})\psi_{el}(\boldsymbol{r};\mathbf{R}), \tag{4}$$

where $\hat{H}_{el}(\mathbf{R})$ can be written as:

$$\hat{H}_{el}(\boldsymbol{r};\mathbf{R}) = h_0 + \Sigma_i\, h_i + \Sigma_{i<j}\, g_{ij}. \tag{5}$$

Terms in $\hat{H}_{el}(\boldsymbol{r};\mathbf{R})$ are the constant nuclear interaction term, h_0 :

$$h_0 = \Sigma_{\mu<\nu}\, Z_\mu Z_\nu / \boldsymbol{R}_{\mu\nu}, \tag{6}$$

the one electron term, h_i :

$$h_i = -\nabla_i^2/2 \; -\Sigma_\mu\, Z_\mu / \boldsymbol{r}_{i\mu}\ , \tag{7}$$

and the two-electron term, g_{ij} :

$$g_{ij} = 1/\boldsymbol{r}_{ij} \tag{8}$$

given in atomic units, where Z denotes atomic number, $\nabla_i^2/2$ is the kinetic energy operator, $\boldsymbol{r}_{\mu\nu}$, $\boldsymbol{r}_{i\mu}$, and $\boldsymbol{r}_{ij}$ are distance between two nuclei, an electron and a nucleus, and two electrons, respectively, and indices i and j run over electrons while μ and ν run over nuclei.

The electronic Schrödinger equation for a system of chemical interest has too many degrees of freedom and further approximations are needed. Two most common approaches are wave function and electron density based methods. The system's energy is minimized by optimization of orbitals in molecular orbital (MO) theory or coefficients of basis orbitals in valence bond orbitals in valence bond (VB) theory in the former case, and by optimization of electron density in the latter case.

1.2.1. Molecular orbital theory methods

The eigenfunctions of a Hamiltonian for an electron moving in a central field, atomic orbitals (AOs), can be expressed as a linear combination of basis functions composing a complete set.[10] Basis sets are usually chosen to mimic the physics of the problem, such as Slater type functions,[11] or to be computationally efficient, like plane waves and Gaussian type functions.[12,13] However, basis functions are non-unique - any complete set of basis orbitals can be used to give AOs of any atom. Molecular orbitals (MOs) are formed as a linear combination of AOs on different atoms and represent eigenfunctions of the one-electron Hamiltonian. The one-electron Hamiltonian, Fock operator (***F***), includes interactions between electrons in a mean-field way. In principle, an MO can contain contributions from any AO of any atom. In semiempirical methods, valence AOs are sometimes transformed into hybrid orbitals, liner combinations of AOs on a single atom, which have electron density concentrated in the direction of chemical bonds; the direction of hybrid orbitals is predicted from anticipated molecular geometry.[14, 15]

A trial wave function is built as an antisymmetrized product of trial MOs filled according to the Pauli exclusion principle,[16] and represented as a Slater determinant.[17] Energy can be calculated using the trial wave function:

$$E_{el}(\boldsymbol{r};\mathbf{R}) = \langle \psi_{el}(\boldsymbol{r};\mathbf{R}) | \boldsymbol{F}(\boldsymbol{r};\mathbf{R}) | \psi_{el}(\boldsymbol{r};\mathbf{R}) \rangle / \langle \psi_{el}(\boldsymbol{r};\mathbf{R}) | \psi_{el}(\boldsymbol{r};\mathbf{R}) \rangle. \quad (9)$$

It is approximated that the total wave function can be represented with one determinant. The goal is to determine the set of MOs for which the energy is at a minimum. This is accomplished by constrained optimization of MOs using Lagrange multipliers within an iterative procedure. The final energy satisfies the variational principle,[18] which states that any approximate wave function will have energy higher or equal to the exact energy. This procedure is called Hartree-Fock (HF) method.[19]

During the optimization, an electron interacts with an averaged density of all other electrons.

The Hartree-Fock method solves all one- and two-electron integrals that arise during the calculation. The next level of approximation is to avoid or simplify the calculation of the integrals, which is done with wave function based semiempirical methods. Semiempirical methods differ in the integral approximation they assume.[20] Semiempirical self-consistent field (SCF) methods focus on the valence electrons, while the core electrons are included throughout reduced nuclear charge or an effective core potential. The values of one-electron integrals are fitted to reproduce experimental data or high-level calculations. Some two-electron integrals are neglected; complete neglect of differential overlap (CNDO) sets to zero all two-electron integrals that depend on the overlap of different basis orbitals (zero-differential overlap (ZDO)[21]) and all one-center two-electron integrals between different orbitals on the same atom; intermediate neglect of differential overlap (INDO) uses ZDO, but calculates one-center two-electron integrals; neglect of diatomic differential overlap (NDDO) calculates one- and two-center two-electron integrals, but ignores the rest.[22] The remaining two-electron integrals are usually calculated from analytical formulas. As in the HF case, the energy of the system is minimized by optimization of the molecular orbitals.

The next level of approximation, neglect of all two-electron integrals, leads to the simplest, non-iterative semi-empirical methods. These methods have two types of one-electron integrals: Coulomb integrals that describe the energy of an electron in the orbital of an isolated atom, and resonance integrals that describe the bonding interactions in the molecule. The goal of these methods is to capture simple underlying physics of electron interactions in a molecule, rather than to give quantitative predictions. The first and the simplest model is Hückel theory, which includes only one AO on each non-hydrogen atom and non-zero resonance integrals only between AOs on atoms that share a bond.[23] It has been used to understand π-electron delocalization. The most general

of the simple models is extended Hückel theory (EHT) which includes all valence electrons and all resonance integrals.[24]

The Hartree-Fock energy is always higher than the exact energy of a system. Part of the energy difference comes from a limited number of orbitals which are used to describe electron motion. However, another part of the difference comes from the approximations made within the HF procedure - a single determinant approach cannot correctly describe systems where two or more determinants are close in energy (static correlation), while the mean-field way the electron-electron interactions are calculated does not describe accurately the Coulomb repulsion between electrons (dynamic correlation).[25,26] Correlation effects can be added to the HF wave-function in different ways.

The configuration interaction (CI) method creates a molecular wave function as a linear combination of the ground determinant and excited determinants where one or more electrons are promoted to higher energy orbitals, and optimizes the coefficients of determinants in the variational SCF procedure.[27] Full-CI calculation includes all possible determinants of correct symmetry and represents the exact solution of the equation 4 for a given basis set. Because full-CI calculations include large number of configurations they are accessible only for small molecules and basis sets. CI calculations are made more accessible for larger molecules by reducing the number of excited determinants included in the wave function. Like the HF energy, an approximate CI energy is always an upper bound of system's energy.

Perturbation theory can be used to correct for missing dynamic correlation. Møller-Plesset (MP) approach is the most used application of perturbation theory in quantum chemistry.[28, 29] MP*n* theory uses a sum of one-electron Fock operators as zeroth order Hamiltonian. The HF wave function is the lowest-lying zeroth-order wave function. Other zeroth-order wave functions are all

possible excited determinants formed from the HF wave function. The perturbation Hamiltonian is the difference between exact and averaged electron-electron interactions. Variational theorem does not hold for perturbation methods and there is no guarantee that the calculated energy is higher than the exact energy. MP*n* theory has been developed up to 6th order in the series expansion, but because of oscillations in higher-order energy corrections and occasional failures of the series to converge the second-order Møller-Plesset perturbation theory (MP2) is mostly used.

1.2.2. Density Functional Theory

Density functional theory (DFT) approaches solve the equation 4 in a different way than the wave function based methods. DFT starts from electron density of a system, which is defined as:

$$\rho(\boldsymbol{r_1}) = N\int|\psi_{el}(\boldsymbol{r},\mathbf{R})|^2 d\mathbf{r}_2...d\mathbf{r}_N \quad (10)$$

where N is the number of electrons in the molecule, $\psi_{el}(\boldsymbol{r},\mathbf{R})$ is the wave function of the molecule, and $\mathbf{r}_2$,..., $\mathbf{r}_N$ are the coordinates of the N-1 electrons. As shown in the first Hohenberg-Kohn theorem, the electron density is a fundamental property of a system, uniquely defined for a given external potential determined by positions and charges of the nuclei, and can be used to calculate other properties, which are expressed as functionals of the density.[30] In the density terms, equation 4 becomes:

$$E[\rho] = V_{nuc\text{-}el}[\rho] + T_{el}[\rho] + V_{el}[\rho] + V_{nuc\text{-}nuc} \quad (11)$$

where $V_{nuc\text{-}el}[\rho]$ is the system-specific interaction between the nuclei and the electron density, $T_{el}[\rho]$ is the kinetic energy, $V_{el}[\rho]$ is the electron-electron interaction energy, and $V_{nuc\text{-}nuc}$ is nuclear-nuclear interaction term. The second Hohenberg-Kohn theorem proves that the variational principle holds if the approximate electron density is used to solve equation 11. The exact electron density for the

system minimizes the energy of the system and it can be obtained by minimizing the energy with respect to density variations.

Functionals used in the DFT calculations are a vital part of DFT that can affect the accuracy of the method. Because electronic kinetic energy is on the order of the total energy,[31] even small errors that arise from using density to calculate it can lead to large total error. Instead, most DFT methods use Kohn-Sham theory.[32] Kohn-Sham (KS) theory introduces orbitals into DFT. Equation 11 becomes:

$$E[\rho] = V_{nuc\text{-}el}[\rho] + T_{KS}[\rho] + J[\rho] + E_{XC}[\rho] + V_{nuc\text{-}nuc}, \quad (12)$$

where $T_{KS}[\rho]$ is the kinetic energy of a system of non-interacting electrons calculated from Kohn-Sham orbitals, φ^{KS}:

$$T_{KS}[\rho] = \sum_i <\varphi_i^{KS}(\boldsymbol{r})|-\nabla_i^2/2|\ \varphi_i^{KS}(\boldsymbol{r})>, \quad (13)$$

$J[\rho]$ is the classical electron repulsion of the electron density with itself:

$$\mathrm{J}[\rho] = (1/2)\int\int(\rho(\boldsymbol{r}_1)\rho(\boldsymbol{r}_2)/\boldsymbol{r}_{12})d\boldsymbol{r}_1 d\boldsymbol{r}_2, \quad (14)$$

and $E_{XC}[\rho]$ is the exchange-correlation energy which represents the difference in energy between the real system and the system of non-interacting electrons.

$$E_{XC}[\rho] = T_{el}[\rho] - T_{KS}[\rho] + V_{el}[\rho] - J[\rho]. \quad (15)$$

Starting from trial KS orbitals and a single determinant wave-function, KS equations:

$$(-\nabla_i^2/2 + V_{nuc\text{-}el}(\boldsymbol{r}) + \delta J[\rho]/\delta\rho(\boldsymbol{r}) + \delta\, E_{XC}[\rho]/\delta\rho(\boldsymbol{r}))\ \varphi_i^{KS}(\boldsymbol{r}) = \varepsilon_i\ \varphi_i^{KS}(\boldsymbol{r}), \quad (16)$$

are solved in an iterative fashion, where the electron density is calculated using:

$$\rho(\boldsymbol{r}) = \sum_i [\varphi_i^{KS}(\boldsymbol{r}))]2. \quad (17)$$

For a system of non-interacting electrons, $\mathrm{E_{XC}}[\rho] = 0$, KS theory can yield exact electron density. If exact form of the exchange-correlation functional is used, it is possible to calculate the exact energy and density for a real system. Unfortunately, the exact form of the exchange-correlation functional is not known, and DFT methods differ in the way that they approximate it.

DFT calculations can be time-consuming and are not commonly used on systems that have more than 200 atoms. Similar to the wave function based methods, the problem of the system size is solved by additional approximations that lead to a density-functional tight-binding scheme (DFTB).[33] DFTB method starts by defining initial density, $\rho_0(\boldsymbol{r})$, as a sum of atomic densities without charge transfer interactions that come from bonding. Only valence electrons are used in the calculation of $\rho_0(\boldsymbol{r})$, and nuclei are substituted with pseudo-atoms. Pseudo-atoms are created from atoms by adding confinement potential to the atomic Hamiltonian and calculating a compact basis composed of valence orbitals. It is assumed that the real density of the chemically bonded system, $\rho(\boldsymbol{r})$, does not differ significantly from $\rho_0(\boldsymbol{r})$, and that real density can be calculated by expanding E[ρ] at $\rho_0(\boldsymbol{r})$ to second order. In the spirit of semiempirical methods, Hamiltonian matrix elements between orbitals, $H_{\mu\nu}^{\ 0}$, are parameters of the method. Atomic charges, Δq_I, are calculated as the difference between Mulliken populations[34] and the number of valence electrons of pseudo-atom, I. The total energy is calculated as:

$$E[\rho]= \Sigma_i f_i \Sigma_{\mu\nu} c_\mu^{\ i} c_\nu^{\ i} H_{\mu\nu}^{\ 0} + (1/2)\Sigma_I \Sigma_J \gamma_{IJ}(\mathbf{R}_{IJ})\Delta q_I \Delta q_J + \Sigma_{I<J} V_{REP}^{\ IJ}(\mathbf{R}_{IJ}) \qquad (18)$$

where f_i is the occupancy of i^{th} orbital, $c_\mu^{\ i}$ and $c_\nu^{\ i}$ are orbital coefficients, $\gamma_{IJ}(\mathbf{R}_{IJ})$ are atomic parameters that determine how easy it is for electron density to fluctuate between pseudo-atoms I and J, and $V_{REP}^{\ IJ}(\mathbf{R}_{IJ})$ is a repulsive pairwise function, which is obtained by fitting. Finally, the energy and density are obtained in a self-consistent calculation, by minimizing $E[\rho]$.

Time-dependent DFT (TDDFT) is used in the calculations of the excited states.[35] The Runge-Gross theorem states that the exact time-dependent density determines the time-dependent potential up to a constant and the time-dependent wave-function up to a phase factor, proving that the time-dependent density is a unique property of a system from which all other properties can be calculated.[36] The total energy is not a conserved quantity in time-dependent systems, and the

variational principle does not hold. TDDFT is based on the conservation of quantum mechanical action - the action of the system is calculated using the action functional acting on a KS density of non-interacting electrons, in self-consistent fashion, until the density converges to the exact density of interacting electrons.[37]

1.2.3. Symmetry

The symmetry of a molecule is defined by the kind and number of symmetry elements such as the center of inversion, axes of rotation, planes of reflection, and roto-reflection axes that the molecule has. The set of symmetry elements in a molecule determines its mathematical (point) group.[38] The molecular Hamiltonian does not change under symmetry operations, as potential energy terms depend only on interparticle distances and the kinetic energy terms are a result of differential operations. This has profound consequences for the physical properties such as dipole moment, and for electronic, vibrational, and rotational transitions.[39] When the Born-Oppenheimer approximation is applied the molecular symmetry is reduced to the operations that leave the nuclear framework invariant. Eigenvalues of one-electron Hamiltonian in the Born-Oppenheimer approximation will belong to irreducible representations of the molecular point group determining the behavior of a state wave function under symmetry operations: when there is a symmetry operation in a molecule, non-degenerate MOs will either be invariant or change sign under it (e.g., if a molecule has a plane of reflection orthogonal to the main axis of rotation, MOs will either be symmetric (σ orbitals) or antisymmetric (π orbitals) with respect to the reflection). The symmetry of MOs determines which AOs can contribute to which MOs.

Even though molecules possess three-dimensional structure they are regarded as zero dimensional systems because they are invariant under translation: molecular coordinates do not repeat when one goes from $\boldsymbol{r}$ to $\boldsymbol{r} + \boldsymbol{R}_{n_1 n_2 n_3}$, where $\boldsymbol{R}_{n_1 n_2 n_3} = (n_1 a_1, n_2 a_2, n_3 a_3)$ is a translational vector. Solids are systems that in addition to the symmetry elements present in molecules, have translational symmetry - whole system can be described by a repeating unit, called unit cell, and three linearly independent vectors, a_1, a_2, a_3, describing how the unit repeats in space. The periodicity can be present in one (polymers), two (layered materials), and three (crystals) dimensions.

In crystals, the periodicity with respect to translation in the real space is reflected in the energy space, where wave vector $\boldsymbol{k} = 2\pi\boldsymbol{m}/N\boldsymbol{a}$, where N is the number of unit cells, $\boldsymbol{m}$ is (m_1, m_2, m_3), and m_i is an integer, has a period of 2π. Usually, the energy space is shown in the first Brillouin zone (FBZ), for $\boldsymbol{m} = (1,1,1)$ and $-\pi \leq \boldsymbol{k} \leq \pi$.[40] When time-reversal symmetry is conserved and $\varepsilon(-\boldsymbol{k}) = \varepsilon(\boldsymbol{k})$, FBZ is plotted only for $\boldsymbol{k}$ from 0 to π. While MOs have discrete energies, periodicity leads to formation of energy bands, regions with a continuous distribution of eigenvalues. They are characterized by the irreducible representation of the band, band minimum (the energy of the most stable of the band's orbitals, $\psi_{\boldsymbol{kmin}}(\boldsymbol{r})$), band maximum (the energy of the least stable of the band's orbitals, $\psi_{\boldsymbol{kmax}}(\boldsymbol{r})$), band width (energy difference between the minimum and the maximum), and the number of states for a unit energy interval (density of states (DOS)). Energy bands are separated by band gaps, regions without eigenstates. Electron eigenstates, crystal orbitals (COs), are given by Bloch's theorem as:

$$\psi_{\boldsymbol{k}}^{\alpha}(\boldsymbol{r}) = \mathrm{e}^{i\boldsymbol{k}\boldsymbol{r}}\, u_{\boldsymbol{k}}^{\alpha}(\boldsymbol{r}), \tag{19}$$

where α is an energy band label, $u_{\boldsymbol{k}}^{\alpha}(\boldsymbol{r})$ is defined as:

$$u_{\boldsymbol{k}}^{\alpha}(\boldsymbol{r}) = \sum_{\mathbf{K}} \tilde{\mathrm{u}}_{\boldsymbol{K},\boldsymbol{k}}^{\alpha}\, \mathrm{e}^{i\boldsymbol{K}\cdot\boldsymbol{r}}\,.^{41} \tag{20}$$

and $\boldsymbol{K}$ are reciprocal lattice vectors. The wave vector determines the nodal structure of COs: $\psi(0, 0, 0)$ the CO has no nodes between unit cells while in $\psi(\pi, \pi, \pi)$ there is a node between all neighboring unit cells.

Helical symmetry is a special case of one-dimensional periodicity that possess rotational symmetry in addition to translational symmetry (Figure 1). As a line, a helix is defined by the helical angle, α, the radius of a helix, ρ, and the pitch a helix, h. In helical polymers, the continuity of a helical line is broken into discrete points corresponding to the positions of atoms in the molecule. The backbone of the helix contains all atoms which are connected through chemical bonds and lie on the imaginary helical line around the main axis of the helix. The parameters of a molecular helix are defined by bond lengths, bond angles, and dihedral angles between backbone atoms.[42] It is possible to define two fundamentally different unit cells: the roto-translational unit cell,[43] which is the smallest possible repeating unit, and the translational unit cell, which contains all atoms in a pitch of a helix.[44,45] When the roto-translational unit cell is used the system is built by a rotation of the unit cell around the helical axis by α degrees and a translation by h/N_1, where N_1 is the number of the roto-translational unit cells needed to make a full turn of 360 degrees. The translational unit cell contains N_1 roto-translational unit cells, and the system is built by a translation by h in the direction of the helical axis. When the translational unit cell is used, the meaning of the wave vector as a reciprocal lattice vector is kept. However, the additional roto-translational symmetry present within translational unit cell introduces symmetry in the FBZ: the bands in the FBZ come in groups of N_1 bands which are connected by inherent degeneracies. FBZ bands can be 'unfolded' into a larger energy zone, called Jones zone,[46] with pseudo wave vector, $\boldsymbol{k'}$ going from $-N_1\pi \leq \boldsymbol{k'} \leq N_1\pi$. The bands in the Jones zone are smooth and the there are no inherent degeneracies.

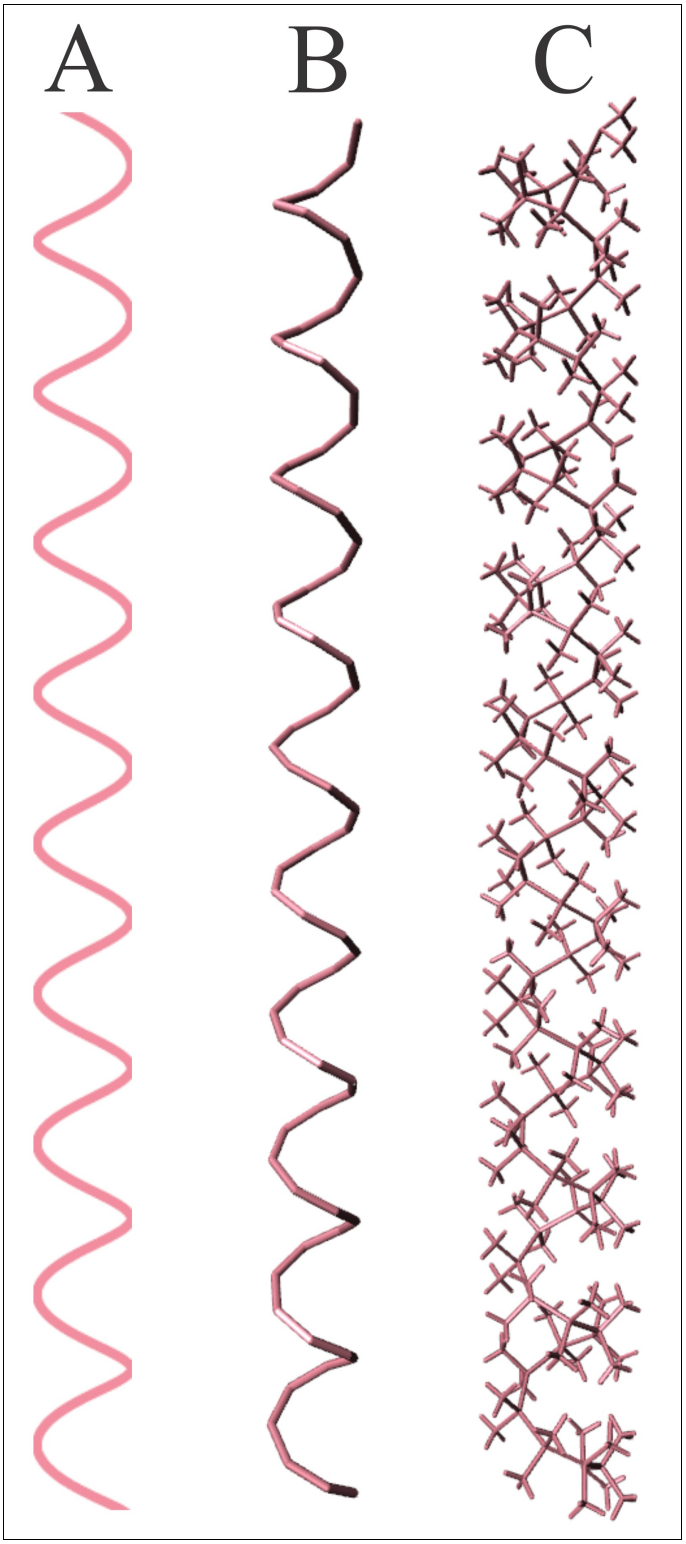


Figure 1. (A) a helix (B) backbone of a molecular helix (C) a molecular helix

1.2.4. Natural Bond Analysis

Once the molecular wave-function is obtained as a liner combination of basis functions or from the electron density, it can be expressed in another set of functions. Natural bond analysis is a way of localizing MOs to give more chemically intuitive description of bonds in a molecule.[47] The analysis starts with a calculation of natural atomic orbitals (NAOs), atomic orbitals that are optimized for a given molecular environment and do not represent the eigenvectors of a spherical atomic Hamiltonian. NAOs differ from AOs in two ways: NAOs are contracted compared to AOs if an atom carries partial positive charge, and more diffuse than AOs if an atom is partially negative; NAOs are orthogonal to all other NAOs, even the ones belonging to different atoms, while AOs on two different atoms are not required to be mutually orthogonal.[48] NAOs are formed in such a way that only valence and core orbitals have significant population, which reduces the effective basis set size. Natural hybrid orbitals (NHOs) are formed as linear combinations of one-center NAOs and are directed along the directions of maximum occupancy (chemical bonds, lone pairs, core electrons).[49] NHOs are used to form natural bond orbitals (NBOs), which can be core NBOs (composed of nearly pure NAO), lone-pair NBOs (composed of nearly pure NHO), or bonding NBOs (linear combinations of two NHOs on atoms that form a chemical bond). Each bonding NBO has a corresponding antibonding NBO. NBOs are not constrained by molecular symmetry. Reverse transformations are also possible - the MOs can be expressed as a linear combination of NBOs.

1.3. σ-Electron delocalization

The abstract concept of the molecular wavefunction is not how chemists usually think about a chemical bond. We think of chemical bonds as electron pairs being shared between two, sometimes three, atoms participating in bonding and represent their structure via Lewis formulas.[50,51,52] These formulas give structural information about bonding in a molecule and show how many electrons are shared between atoms: one shared electron pair gives a single bond; two electron pairs give a double bond, etc. Lewis structures are a simplified model of more complex reality correctly described by a full molecular wave function. NBOs can be thought of as the bridge between the wave function image and the Lewis formulas, where NHOs constructively interfere to form NBOs that are localized in the space between two atoms forming a bond and the ground state wave function is expressed in the basis of these orbitals, but there are also unoccupied antibonding orbitals corresponding to the breaking of the bonds due to destructive interference. If there are two or more Lewis structures that can be written for the same molecule, the ground state wave function cannot be described with an unique set of localized NBOs because electron pairs are shared between more that two nuclei. The molecule is instead represented with multiple Lewis formulas, resonance structures, that represent different possible arrangements of bonds.

The simple idea of shared electron pairs does not account for the fact that bonding will occur whenever there is a constructive interference between two atomic wave-functions. The interference is not limited only to neighboring atoms that share electron pairs, even though the strength of interaction falls off with the distance between atoms. It leads to electron delocalization: a quantum mechanical effect that originates in stabilizing, constructive interference between several atomic centers and leads to a decrease of the total system energy. Electron delocalization arises as the

difference between our simplified models represented in Lewis structures and real molecules described by the exact wave function. It originates in our need to connect the models with reality, and explain discrepancy between predictions of models and real molecular properties.

In molecules that have multiple resonance structures, the delocalization gives us a way to connect different structures and explains increased stability of these systems. The most famous example of electron delocalization in molecules with more than one important Lewis structure is the delocalization in benzene and other acenes that leads to aromaticity.[53,54] The delocalization in acenes reaches its maximum in graphene, a perfectly conductive semi-metal that can be thought of as composed of infinite number of benzene rings fused together.[55] Electron delocalization is present even in systems that can be correctly described with one Lewis structure. For example, the delocalization of electrons in linear polyenes, unsaturated hydrocarbons with alternating double and single bonds, is the cause of their planarity.[56] In acenes and polyenes, the delocalization of π-electrons determines the molecular properties such as reactivity, absorption spectrum, and conductivity.

Molecules do not need to have double bonds and π-electrons to show effects of delocalization. σ-Electron delocalization is present in all molecules that have more than one covalent bond. In peralkylated linear polysilanes the delocalization of σ-electrons affects molecular properties such as charge and electron transfer, optical properties, molecular conductivity, reactivity, and spin density propagation.[57,58] Because σ-delocalization usually involves at least two orbitals per atom there can be different kinds of interference: the delocalization that originates from interference between orbitals at the same center is called σ-conjugation, and the one originating from the interference between orbitals on neighboring atoms that are not included in the formation of a bond between them is known as σ-hyperconjugation. The constructive interference between orbitals on

non-neighboring atoms gives rise to σ-homoconjugation, which is usually weak.[6] The interactions can combine in different ways, leading to either delocalization or localization of electrons in a σ-bonded molecule.

Peralkylated linear polysilanes are used as model compounds for σ delocalization. Unlike saturated hydrocarbons, they absorb in the near UV which makes experimenatl studies of delocalization accessible under standard conditions. Furthermore, due to smaller electronegativity of Si compared to C and H, Si-Si bonds are higher in energy than Si-C or Si-H bonds and the effects of electron delocalization through silicon backbone determine the behavior of the molecule, similarly to the π-electrons in polyenes and acenes. The interference between orbitals on different atoms depends on the overlap between them, which is the cause of the strong conformational dependence of delocalization in silanes.

1.3.1. Models for σ-electron delocalization

In saturated systems, such as silanes, the valence orbitals on each heavy atom are well represented as sp^3 NHOs. As the delocalization depends strongly on the orbitals in the backbone of a linear oligosilane, only NHOs that are included in the formation of backbone bonds can be included in a crude model. This line of reasoning gives two simplest models for σ-electron delocalization, Sandorfy C and Ladder C models (Figure 2), which have two hybrid orbitals on the backbone atoms in the middle of a chain and one hybrid orbital on the backbone atoms at the ends of a chain.[5,59] More complex models, Sandorfy H and Ladder H, include all four valence orbitals on the backbone atoms and one orbital on each lateral substituent. All orbitals are described with Coulomb integrals that correspond to an isolated atom and are determined by the atom's electron

affinity and ionization potential. In Sandorfy models, the interactions between NHOs are described via primary resonance integrals, which determine the strength of the chemical bond, and geminal resonance integrals, determining the strength of interaction between orbitals on the same atom. Sandorfy models do not show conformational dependence, which is added to Ladder models through vicinal resonance integral, which describes the strength of an interaction between two orbitals on neighboring atoms that are not included in the primary bonding betweene these two atoms. Unlike primary and geminal resonance integrals, vicinal resonance integral changes sign as the backbone dihedral angle goes from 180° to 0°.

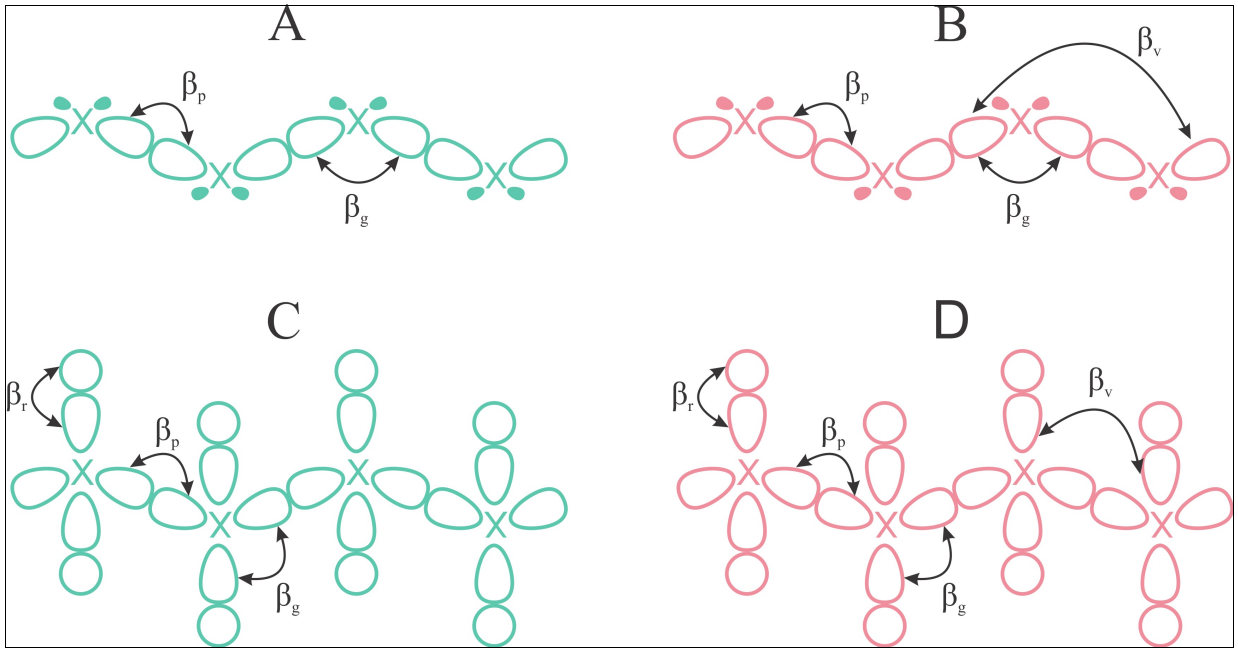


Figure 2. (A) Sandorfy C (B) Sandorfy H (C) Ladder C (D) Ladder H

1.3.2. Quantifying electron delocalization

Electron delocalization is not an observable and cannot be measured experimentally. It manifests itself only through effects it has on the properties of molecules, e.g. the delocalization of π-electrons in polyenes and σ-electrons in planar linear oligoslianes give rise to red-shifted absorption. Experimentally, the effects of delocalization are judged from magnetic properties like NMR chemical shifts and changes in magnetic susceptibility,[60,61] optical properties like UV spectra and symmetry in Raman spectra,[62,63] thermochemical stability of molecules,[64] or structural changes like equalization of lengths of single and double bonds.[65]

An exact theoretical measure of electron (de)localization does not exist, but there are many ways of approximating the extent of delocalization in molecules. Number and stability of resonance structures of a molecule could be used to indicate presence of delocalization.[66] Analysis of the electron density of a system, which can be calculated from the wave function, can be a helpful tool in an analysis of delocalization.[67] Most commonly used density based methods, such as atoms in molecules (AIM)[68,69] and electron localization function (ELF),[70,71] are based on the two-electron density, or pair density. All these methods rely on the knowledge of the full molecular wave function.

As the goal of this thesis is to explain the conformational dependence of σ-electron delocalization in intuitive terms connected to the structure and nodal patterns of frontier orbitals, we turn to simpler methods to approximate electron delocalization. In molecules, we use partition ratio, p_i, of a normalized MO i as a measure of the delocalization of an electron or hole in that orbital. The partition ratio is defined as:

$$p_i = 1/(m \sum_{\mu=1}^{\mu=m} c^4_{\mu i}) \,, \tag{21}$$

where m is the number of sites and $c_{\mu i}$ is the amplitude of orbital i on site μ.[72] When all coefficients have the same magnitude, $p_i = 1$ and the orbital is perfectly delocalized. Likewise, when an orbital is perfectly localized on a site, $\mu = n$, $c_{ni} = 1$, $p_i = 1/m$.[73]

When crystal orbitals are described as linear combinations of plane waves p_i is 1 and the partition ratio cannot be used as a measure of delocalization. The bandwidth of a valence or a conduction band can indicate the strength of interactions between sites: when atoms on different sites interact strongly the bandwidth increases and electrons can easily move between sites; when there is no communication between sites the bandwidth goes to zero and electrons are localized on a single site. A useful measure of the ease with which electrons can move between sites is the effective electron and hole mass, calculated from the band structure. Effective mass depends on the density of states near the top of the valence or the bottom of the conduction band, and it is connected to the bandwidth. The position of the band maximum or minimum in reciprocal space can be used to connect the delocalization in molecules and crystals, as frontier MOs correspond to the COs at the valence band maximum and the conduction band minimum.

1.4. Oligosilanes

Oligosilanes are saturated silicon analogues of hydrocarbons. Even though their Lewis structures are identical and preferred ground state geometries are similar, there are differences between these compounds, rooted in significantly larger electronegativity of carbon: while electronegativity of C and H is similar and C-H bonds are only slightly polarized, Si-H and Si-C bonds are polarized towards H or C due to the smaller lectronegativity of Si. The diference in electronegativity leads to energy separation between Si-Si and Si-H (Si-C) bonds. The frontier

orbitals of longer oligosilanes are usually σ-symmetry orbitals located along the backbone, which facilitates the interpretation of the absorption spectra as well as the modeling of the delocalization.

Alkylation of oligosilanes increases their stability, and peralkylated oligosilanes are preferred to the hydrogen analoges in experimental studies. However, introduction of alkyl groups also changes their stable geometries: the alkane-preferred dihedral angle of 180° decreases to values around 165° due to the steric interactions; the *gauche* minimum at 60° in alkanes splits into *ortho* minimum at 90° and smaller *gauche* minimum at around 55°. This thesis will use standard nomenclature for the structural conformations based on silicon backbone dihedral angle (Figure 3).[74]

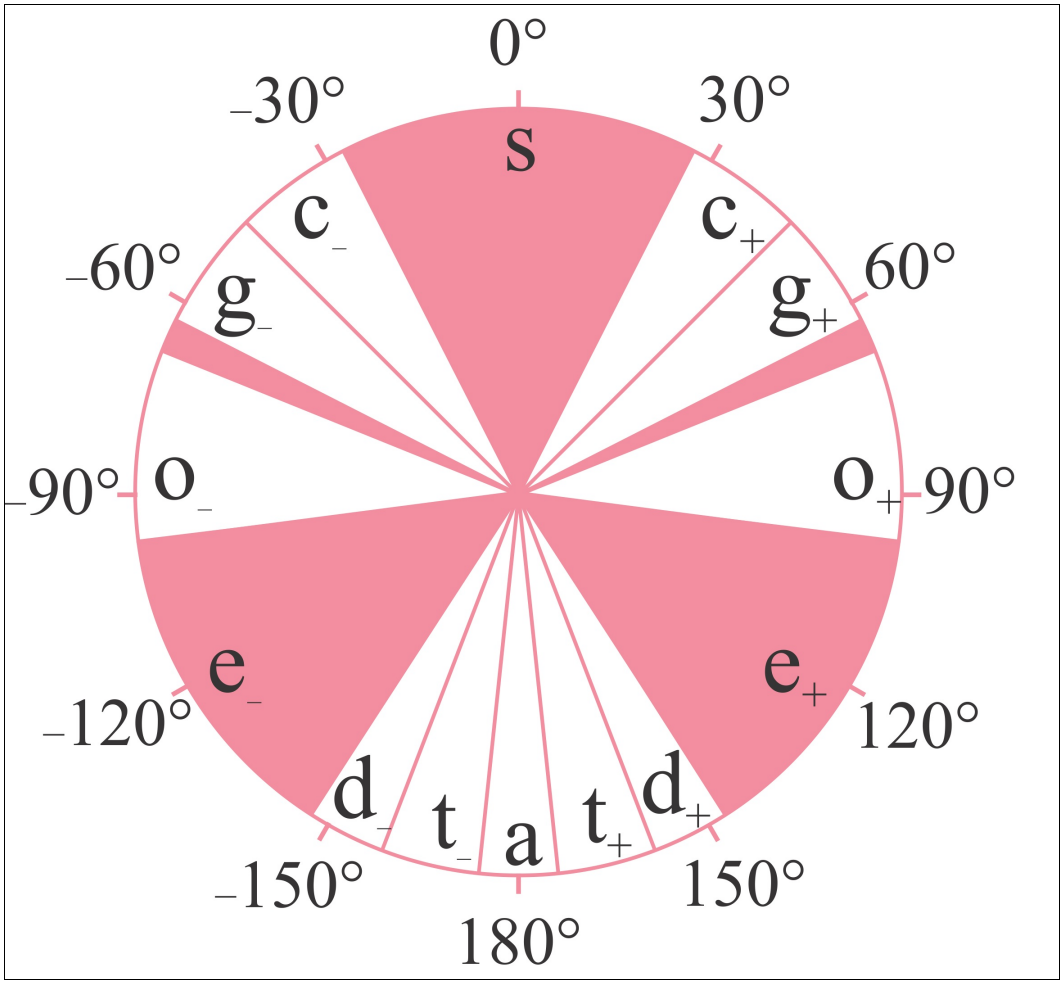


Figure 3. A graphical representation of silicon backbone dihedral angles.

Chapter II

Intuitive Understanding of σ Delocalization in Loose and σ Localization in Tight Helical Conformations of an Oligosilane Chain[1]

2.1. Introduction

The effects of σ-electron delocalization dominate optical properties of σ-bonded structures and extend to many others, such as ionization potential, charge and energy transfer, spin density propagation, and chemical reactivity. A striking example is provided by the optical properties of peralkylated linear polysilanes, fully saturated chains with an all-silicon backbone.[2,4,75,76] The delocalization is sensitive to backbone conformation and leads to phenomena such as thermochromism,[77,78,79,80,81] piezochromism,[82,83] electrochromism,[84] ionochromism,[85,86] and solvatochromism.[87] Also, the single-molecule electrical conductivity of oligosilanes appears to depend on conformation.[58] In long polysilane chains conformational segmentation into individual chromophores is important for optical absorption, emission, and charge transport properties.[5,88,89]

The effect of backbone conformation on the electronic excitation energies of peralkylated oligosilanes is nicely illustrated by the stark contrast between the reported effects of chain-length extension in chains kept in an all-transoid conformation [*t*] and those held in an alternating cisoid,anti conformation [*ca*] (Chart 1; in either measurement, the sense of chain helicity varies randomly along the chain). As shown in Figure 4, an extension of the SiSiSiSi backbone from four

[1] Adapted with permission from Jovanovic, M., Antic, D., Rooklin, D., Bande. A., Michl, J. *Chem. Asian J.* **2017**, *12*, 1250 -1263. (Copyright © 2017 by John Wiley Sons, Inc.)

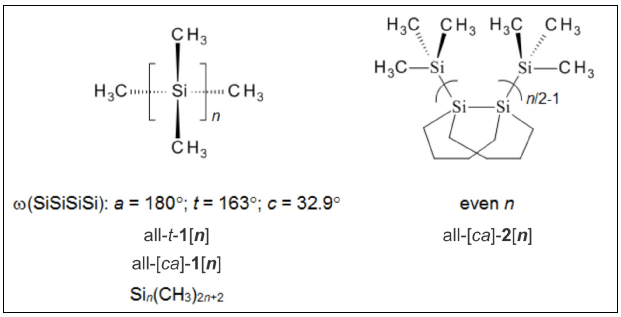


Chart 1. Structural formulas of peralkylated oligosilanes.

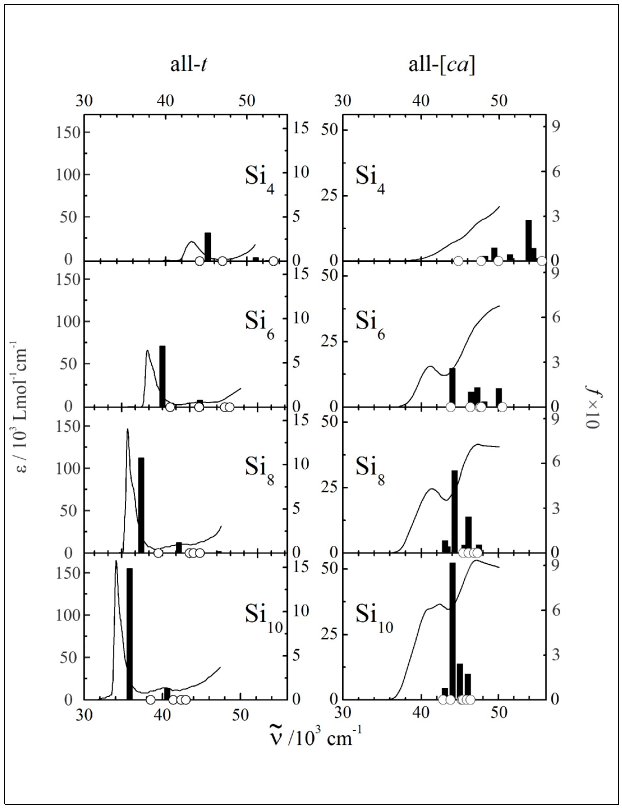


Figure 4. Absorption spectra and calculated ten lowest singlet-singlet transition energies and oscillator strengths (TD B3LYP/TZ, gas phase). Left: measured for all-$t_{\pm}$-**1[*n*]** (n = 4 - 10) in cyclopentane-isopentane (3:7 v/v) at 77 K and calculated for all-t_{+}-**1[*n*]**. Right: measured for all-[$c_{\pm}a$]-**2[*n*]** in tetrahydrofuran at room temperature, and calculated for all-[$c_{+}a$]-**1[*n*]**. Reprinted with permission from ref. 21. Copyright 2003 American Chemical Society

to ten silicon atoms lowers the excitation energy of the first σσ* excitation by 9 000 cm^{-1} (232 to 293 nm) in the former case,[90] whereas in the latter, it makes no difference at all, and the excitation energy remains steady at ~41000 cm^{-1} (~243 nm).[91] The results are well reproduced by TD B3LYP/TZ//MP2/TZ calculations (TZ ≡ 6-311G**).[4,92]

The contrast shown in Figure 4 provided the motivation for the present study, in which we consider the particularly simple optimized regularly helical oligosilane conformations with all backbone dihedral angles nearly identical. We use this vehicle to address the general issue of conformational dependence of σ delocalization, and particularly the widespread feeling that all-anti saturated chains σ-delocalize best, whereas gauche kinks in the chain hinder delocalization. Our computations rely primarily on the TD B3LYP/TZ method, which reproduces conformational effects on oligosilane electronic spectra. Our ultimate objective, simple

intuitive understanding of the origin of the difference between "σ-delocalized" and "σ-localized" conformations, is achieved by the use of simplified models that successfully reproduce the properties obtained from all-electron calculations for the highest occupied molecular orbital (HOMO). In the molecular orbital (MO) approximation, the HOMO determines the ionization potential and the distribution of positive charge when the chain is doped with a hole, and the dependence of its properties on the chain length provides a reliable measure of the degree of σ delocalization. We use the Hückel Ladder H (considering four hybrids on each silicon atom and one on each hydrogen or alkyl substituent) and the even simpler Ladder C (considering only the two backbone-building hybrids on each silicon) models for closer examination, and find that an inspection of wave functions in both conformational limits, "loose helix" at ω = 180 and "tight helix" at 0°, provides an especially informative view.[5,93,94] In reality and in DFT or Hartree-Fock (HF) calculations, steric hindrance prevents us from reaching the tight-helix all-syn limit ω = 0° for $n > 4$, but in the Ladder models, it does not. Finally, we note that the Ladder C model is already known to account for the strong effect of conformation on the red shift of the σσ* transition that is induced by doubling the number of SiSi bonds in an oligosilane (the attribution of σ and π character to MOs of a saturated chain is discussed below).[6] A similarly simple procedure is currently not available for σπ* transitions.

We use permethylated oligosilanes rather than the unsubstituted parent oligosilanes (all-ω-Si_nH_{2n+2}), likely to reveal the same principles, because we want to compare our results with already published experiments on helices in which the degree of helicity is regular (but its sense random). Unlike the perfectly stable peralkylated oligosilanes for which much information is available, the parent oligosilanes are unstable, pyrophoric, and rarely studied.[95]

2.2. Methods

Chart 1 displays the structural formulas of the oligosilanes of interest. Structures all-*t*-**1[4]** to all-*t*-**1[16]** represent the regular helical geometries of the all-*t*-Si_nMe_{2n+2} permethylated oligosilanes with a backbone dihedral angle ω ≈ 163° along the entire chain length and are dealt with presently. The structures [*c*]-**2[4],** all-[*ca*]-**2[6],** all-[*ca*]-**2[8]**, and all-[*ca*]-**2[10]** have alternating SiSiSiSi backbone dihedral angles ω and ω', where the cisoid angle is constrained to ω = 32.9° and the anti angle to ω' = 180°, and are not a subject of the current study. Both sets of structures are defined as regular helices with chain lengths n = 4 - 16 and 4 -10, respectively (the samples for which experimental data are available undoubtedly have a random distribution of helical sense along the chain).

The ground state geometries of all-*t*-**1[2*m*]** (m = 2 - 8) and all-*t*-**1[2*m*+1]** (m = 2 - 4) were optimized at the MP2/6-311G** (TZ) level of theory subject to the angular constraints stated, using the RI approximation in the Turbomole program package.[96] In our past experience, MP2 optimized and DFT optimized geometries are very similar, but when it comes to dihedral angles, the former agree a little better with experiment, presumably because they include dispersion interactions. We use MP2 geometries but expect that the conclusions would not change if we used DFT geometries instead.

Geometries of other nearly regularly helical ground-state conformations of linear permethylated oligosilanes of chain lengths extending from n = 4 to n = 16 were optimized at the same level of theory. This caused the dihedral angles within the same molecule to deviate by 1 - 2° from each other, and we checked that this made no difference in the results. Optimized conformers exhibiting nearly regular helical patterns along the silicon backbone were all-gauche (*g*; ω ≈ 55°),

all-ortho (*o*; ω ≈ 90°), all-eclipsed (*e*; ω = 120°), all-deviant (*d*; ω = 150°), all-transoid (*t*; ω ≈ 163°), and all-anti (*a*; ω = 180°).[74] For $n = 16$, we also optimized the all-cisoid conformation (*c*; ω ≈ 37°). From earlier work,[84,85,87,90] the *g*, *o*, and *t* conformations at internal SiSi bonds are known to represent local minima on the potential energy surfaces of short permethylated oligosilanes, and chains substituted with longer alkyls occasionally show additional minima at *c* and *d* conformations. The optimization of the *e*, *d*, and *a* conformations, which do not correspond to minima in the potential energy surface of permethylated oligosilanes, was constrained in that the dihedral angles were set equal to the values specified above. Odd-numbered chain lengths from $n = 5$ to $n = 15$ were constructed by extending the optimized even-numbered chains by one trimethylsilyl group at the proper dihedral angle ω, and the resulting geometries were symmetrized prior to performing single-point energy calculations at the HF/6-311G** (HF/TZ) and B3LYP/6-311G** (DFT/TZ) levels, using Gaussian 03W.[97]

Excitation energies and oscillator strengths were calculated by the TD DFT (RPA) procedurec using the B3LYP/TZ (TD DFT/TZ) method in the Gaussian 03W or Gaussian 09 program suite.[98, 99] TD DFT (TDA) results were also obtained for all six conformations of Si_8Me_{18} and were virtually identical, with excitation energies differing by less than 0.05 eV, oscillator strengths by less than 20%, and the amplitudes of various electron promotions by less than 2%. NHOs of all molecules were calculated using the Gaussian NBO versions 3.1 and 5.0.[100,101] The amplitudes of MOs in the NHO basis were used to compute percent σ and π character of an MO according to published formulas,[6] modified slightly as described belowe. The percent σσ* and σπ* character of an excitation was determined as a weighted average of σσ* and σπ* contributions provided by each MO pair contributing to the excitation, respectively.

A modification of the original procedure for determining the percent σ and π character of a molecular orbital that has been introduced presently changes only the contributions provided by terminal $SiMe_3$ groups. It makes the definition more compatible with standard usage for chains whose backbone can achieve planarity. Now, not only all of the *A* symmetry, but also half of the *E* symmetry contribution of terminal $SiMe_3$ counts toward σ character, while the other half of the *E* symmetry contribution counts toward π character. To achieve this, equations (12) in ref. 6 have been modified from the original

$$s_{\kappa,\lambda} = s_{\kappa,\lambda'\lambda''\lambda'''} = c_{\kappa A2}/(c_{\kappa A2} + c_{\kappa E1}{}^2 + c_{\kappa E2}{}^2) \tag{22}$$

$$p_{\kappa,\lambda} = p_{\kappa,\lambda'\lambda''\lambda'''} = (c_{\kappa E1}{}^2 + c_{\kappa E2}{}^2)/(c_{\kappa A2} + c_{\kappa E1}{}^2 + c_{\kappa E2}{}^2) \tag{23}$$

to the newly adopted

$$s_{\kappa,\lambda} = s_{\kappa,\lambda'\lambda''\lambda'''} = (c_{\kappa A2} + c_{\kappa E1}{}^2)/(c_{\kappa A2} + c_{\kappa E1}{}^2 + c_{\kappa E2}{}^2) \tag{24}$$

$$p_{\kappa,\lambda} = p_{\kappa,\lambda'\lambda''\lambda'''} = c_{\kappa E2}{}^2/(c_{\kappa A2} + c_{\kappa E1}{}^2 + c_{\kappa E2}{}^2) \tag{25}$$

Excitation energy surfaces of regular oligosilane helices Si_nMe_{2n+2} were plotted as a function of chain length *n* and backbone SiSiSiSi dihedral angle ω and their color indicates either the oscillator strength per Si atom, *f/n*, or the percent of σσ* character. They were obtained by spline interpolation between the grid points for which calculations were performed, using a 6° mesh size. The color mapping of the surface was handled automatically within Matlab® by linear interpolation along the two directions of the surface plane.[102] The surrounding grid points were assigned a value of the RGB code.

The parameters used in the Hückel calculations were (in eV): Ladder C, α_{Si} = -6.1, β_p = -3.5, β_g = -1.1, β_v = 0.11 - 0.70×cosω; Ladder H, α_{Si} = -6.5, α_C = -9.6, β_p = -3.2, β_{SiR} = -3.8, β_g = -1.8, β_v = -0.28 - 0.99×cosω.[5] The presence of partial *s* character in the NHOs causes the dependence of β_v on ω to be less symmetrical than the usual angular dependence of the overlap of two pure *p* orbitals.

In the calculation of the partition ratio p_i of a molecular orbital i in the Ladder C model the m sites are identical with the m members of the NHO basis set.

2.3. Results

2.3.1. σ-Delocalized and σ-Localized Conformers

The left-hand side of Figure 4 compares the low-temperature UV absorption spectra of the linear permethylated oligosilanes Si_nMe_{2n+2} (n = 4, 6, 8, and 10),[92,103,104,105,106,107,108,109] believed to be due to the all-*t* conformers with a randomly distributed helicity sense,[4] with the transition energies and oscillator strengths calculated (TD DFT/TZ) for the all-*t* conformers all-*t*-**1[4]** to all-*t*-**1[10]**. The only observed intense absorption maximum gradually shifts from 43 100 cm^{-1} in Si_4Me_{10} to 34 100 cm^{-1} in $Si_{10}Me_{22}$, and gains a factor of nearly 10 in intensity in the process. The long-axis polarized excitations to the first and only calculated strongly allowed excited state of *B* symmetry are in good agreement with the positions of the intense bands apparent in the observed absorption spectra. All calculated energies are slightly too high (perhaps due to neglect of solvent effects). A series of much weaker additional transitions is calculated to be present. Only one of them has significant intensity and is actually observed, while the rest would not be expected to be easily detectable. In peralkylated *n*-tetrasilanes, whose spectra have been studied in considerable detail at a series of conformations, these additional transitions have been uncovered and are in impressive agreement with the results of TD DFT/TZ, CAS-PT2, and SAC-CI calculations.[4,91,94] A less detailed study is available for a few conformers of peralkylated hexasilanes.[110]

The right-hand side of Figure 4 serves only for highlighting the contrast between a σ-delocalized and a σ-localized behavior. It displays the reported UV absorption spectra of the alternating polycyclic oligosilanes all-[*c*]-**2[4]** to all-[*ca*]-**2[10]**),[91] again with a randomly distributed helicity sense, in which the purpose of the additional alkane chains is to impose on the silicon backbone the geometry of the desired conformation. Along with these spectra, Figure 4 shows the results of TD DFT/TZ calculations for the permethylated linear analogues of the these polycyclic oligomers ([*c*]-**1[4]** to all-[*ca*]-**1[10]** in Chart 1, with uniform helical sense). In this series of oligosilanes, there is no red shift in the observed primary absorption maximum with increasing chain length and it remains near 41 000 cm^{-1} ([*c*]-**2[4]** is not a true member of the series since it has only one backbone dihedral angle). The results of the calculations reproduce the observed absence of a trend well, but all calculated excitation energies are too high.

Regular Helical Oligosilanes. Figure 5 shows the TD DFT/TZ surfaces of excitation energy from the 1*A* ground state to the four lowest-lying singlet excited states of permethylated C_2 symmetry oligosilanes as a function of the number *n* of Si atoms in the chain and of the SiSiSiSi backbone dihedral angle ω. Plotting against 1/*n* instead of *n* permits a nearly linear extrapolation of the rapidly dropping energy of the 1*B* transition to $n = \infty$. Higher energy calculated transitions are not considered reliable because of the intervention of Rydberg states and are not shown. In the following, we describe the calculated excitations approximately, using the TD DFT excitation amplitudes, since this is adequate for our purposes. The starting MO for all electron promotions involved in the transitions shown is of σ character, but the terminating orbital can be mostly σ*, mostly π*, or strongly mixed. The color of each surface in Figure 5 reflects the calculated percent σσ* character of the transition. The σσ*/σπ* character of the excited state is strongly mixed at most points in the (ω,*n*) space.

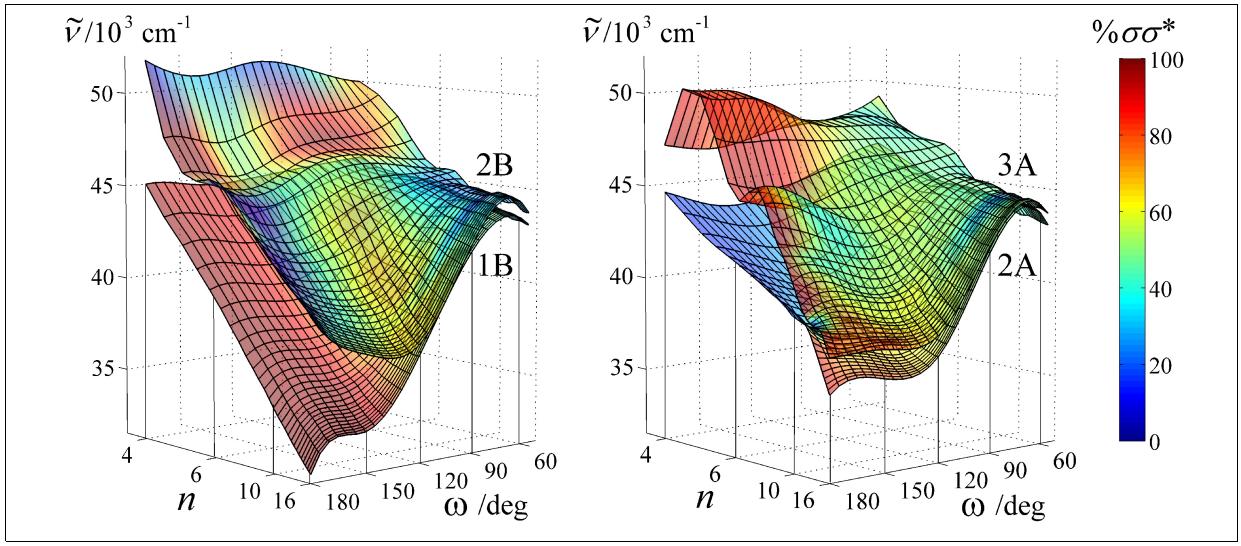


Figure 5. TD DFT B3LYP/TZ transition energy surfaces of the four lowest lying singlet excitations in all-[ω]-**1[*n*]** (*n* = 4 - 16). Left, states of *B* symmetry, right, states of *A* symmetry. The color scale indicates the percent σσ* character of the excited state.

Figure 6 shows the same plot in which color is used to show the computed oscillator strength. Only some transitions into states of *B* symmetry have significant intensity and those into *A* states are all very weak. The intensity is associated with the weight in the excitation of that σσ* promotion

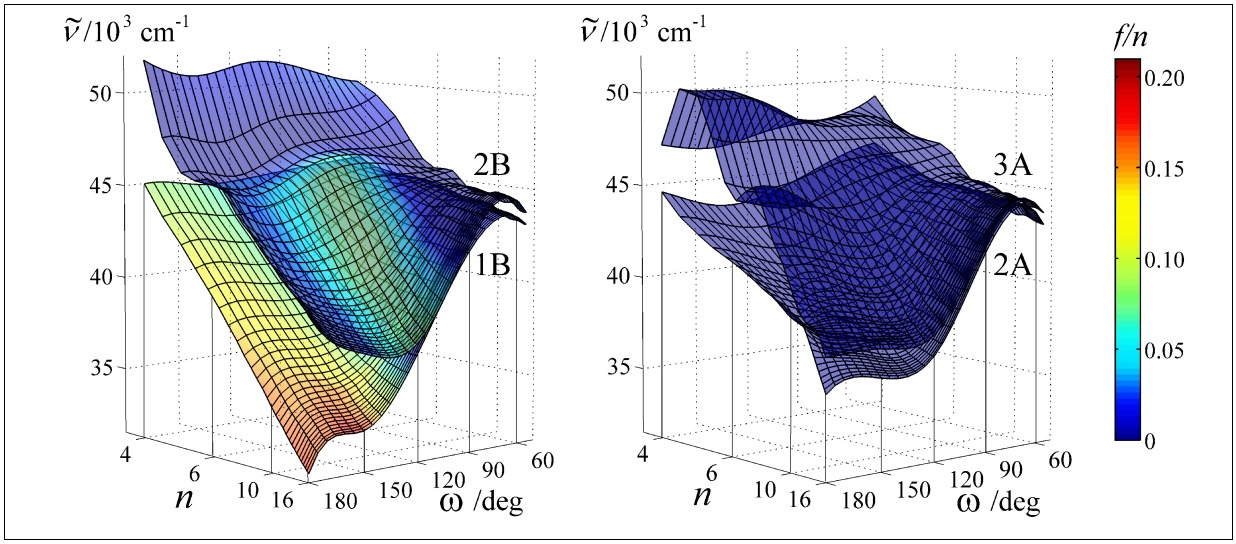


Figure 6. TD DFT B3LYP/6-311G** transition energy surfaces of the four lowest lying singlet excitations in all-[ω]-1[*n*] (*n* = 4 - 16). The color scale indicates the transition oscillator strength per Si atom, *f*/*n*

in which σ and σ* resemble the HOMO and the lowest energy virtual σ* MO at ω = 180° (see below). At ω values close to 180°, this promotion contributes almost exclusively to the transition to the 1*B* state, which completely dominates the spectrum. Transition into the 2*B* state is of the σπ* type and is forbidden at ω = 180°. The only higher transition with noticeable intensity is a weak one into the 3*B* state, faintly seen in the absorption spectrum in Figure 4.

When ω is decreased below ω = 180°, σ*/π* mixing becomes allowed and provides increased intensity to the transition to 2*B* until ω reaches about 120°, at which point the excitation is well described as HOMO to LUMO+2. At smaller dihedral angles the intensity drops again to negligible values. In general, however, only relatively small changes occur upon going from 180° to 120° and in particular, the 1*B* state keeps its HOMO to σ* character and high intensity almost intact. The slope of $E(1B)$ against $1/n$ is gradually reduced; whereas the value of $[dE(1B)/d(1/n)]_{n=\infty}$ at 180° is 72.3×10^3 cm^{-1}, at 163° it is 62.2×10^3 cm^{-1}, at 120° it is 41.7×10^3 cm^{-1}, and at 90° it is only 16.1×10^3 cm^{-1}.

Below 120°, the picture changes entirely (Figures 5 and 6). The 1*B* state loses its σσ* character and becomes predominantly σπ*, while the σσ* character moves to the 2*B* state. The energy of all four computed transitions increases to values characteristic of the shortest chains, and it becomes essentially independent of chain length. At ω values below 90°, the energy of the 1*B* transition drops only up to $n = 6$ and then remains nearly constant in longer chains. None of the four lowest transitions have significant intensity. This has a dramatic effect on the appearance of the calculated absorption spectra, as is illustrated for $Si_{13}Me_{28}$ in Figure 7 (the peak half-width at half maximum, 700 cm^{-1}, was chosen to fit roughly the shape of low-temperature spectrum of all-*t*-**1[10]**[91]). Down to 150°, the transition to the 1*B* state is the strongest, but at 120°, it already only appears weakly and 2*B* with 3*B* carry far more oscillator strength. The trend continues, and the

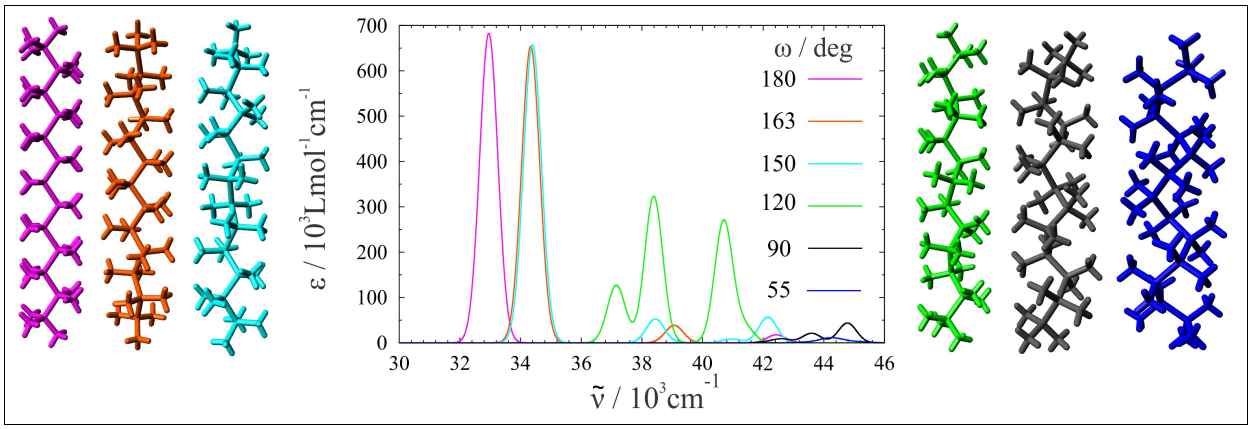


Figure 7. TD DFT B3LYP/TZ absorption spectra of all-*a* (pink), all-*t* (orange), all-*d* (light blue), all-*e* (green) all-*o* (black), and all-*g* (dark blue) conformers of $Si_{13}Me_{28}$. The all-*t* spectrum was shifted by 100 cm^{-1} to lower energies in order to avoid excessive overlap with the all-*d* spectrum.

calculated absorption spectra of all-*o* and all-*g* conformer do not show any intense absorption at low energies. The increase in the energy of the 1*B* transition, the gradual shift of oscillator strength to higher energy transitions, and the reduced separation between transitions as ω decreases are striking.

Figures 5, 6, and 7 demonstrate that regular helical permethylated oligosilanes occur as two entirely different limiting chromophores, one with a loose helix (ω close to 180°) and one with a tight helix (ω close to 0°). As the two are interconverted, their properties correlate smoothly through avoided crossings at ω = 90 - 120°.

The difference between the two limits is in the very different degree of delocalization of the HOMO, which is always predominantly of σ character. Like all other σ(SiSi) bonding MOs, it has no nodes between Si neighbors at any ω. However, it has a node at each of them, since after all, it is the least stable of all σ(SiSi) orbitals. The contrast between the two limits is seen in Figure 8, which shows the standard representation of the HOMO of $Si_{12}Me_{26}$, and much more clearly in the symbolic representation of the HOMO of $Si_{16}Me_{34}$ on the top of Figure 9. The all-anti HOMO is evenly distributed over the whole oligosilane chain and in that regard is reminiscent of the π HOMO of a long polyene. Near the all-syn limit the HOMO consists of a series of islands of large amplitude

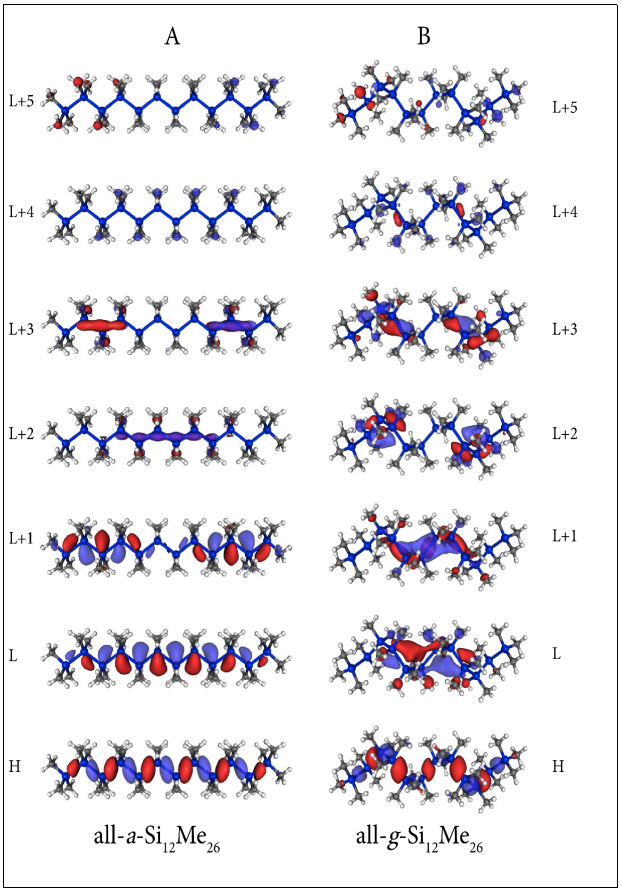


Figure 8. TD DFT B3LYP/TZ frontier orbitals in all-[*a*]-**1[12]** (A) and all-[*g*]-**1[12]** (B).

separated by regions of almost vanishing amplitude, and is reminiscent of those polyene MOs whose energies lie at the center of the bonding π-orbital band. Near the all-syn limit, the energies of electronic excitations in long chains therefore still only reflect those within an individual isolated island. As the chain is built by a gradual increase of *n*, the islands in the HOMO of a tight oligosilane are formed one after another. The delocalization within the first island is reflected in the response of the properties of the shortest oligosilanes to increasing *n*, but the addition of further islands

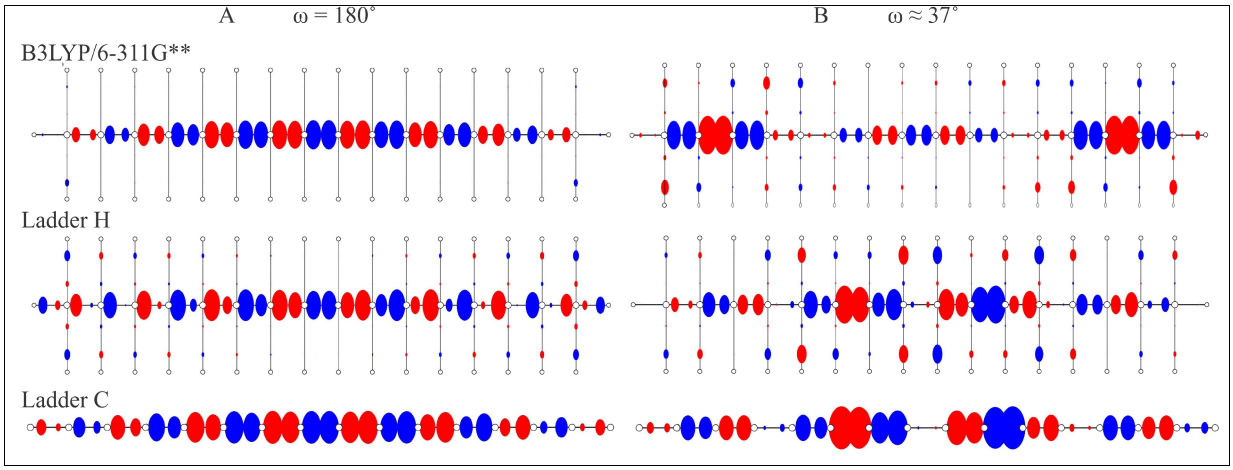


Figure 9. Symbolic representation of the HOMO of all-[ω]-$Si_{16}Me_{34}$ in its all-anti (A) and all-cisoid (B) conformations at three levels of approximation. Larger (smaller) empty circles stand for Si atoms (lateral substituents). Amplitudes (signs) of NHOs are shown by size (color) of ovals located next to the Si atoms and below or above the lateral substituent atoms.

makes little difference (Figure 5). The exact size of the islands into which the HOMO is divided depends on *n* and the details of the calculation, and the reason for this sensitivity will become clear below.

Loose-Helix Oligosilanes. With the present definition of percent σ and π character, at planar ω = 180° geometries symmetry requires each state to be either 100% σσ* or 100% σπ*. The form of the MOs involved in low-energy transitions is illustrated in Figure 8A on the example of all-*anti*-$Si_{12}Me_{26}$. The σ HOMO is the least bonding combination of σ(SiSi) bond orbitals, with geminally (σ-conjugatively) and vicinally (σ-hyperconjugatively) destabilizing nodes at every Si atom, whereas σ* is the most bonding combination of σ*(SiSi) antibond orbitals, with geminally and vicinally stabilizing interactions at every Si atom. The σ* LUMO+1 orbital contains a node at the central Si atom. The two π*(SiC) orbitals, LUMO+2 and LUMO+3, are formed by π interactions of out-of-phase combined SiC antibonds at each Si atom. The more stable LUMO+2 contains no nodes other than the one in the plane of the Si atoms, whereas the less stable LUMO+3 contains an additional node through the central SiSi bond. As usual, the amplitude of these orbitals is concentrated away from nodes. Inspection of the orbital shapes makes it very obvious why only the HOMO to LUMO excitation carries large oscillator strength.

The electronic spectra of the loose helix conformers are characterized by two low-energy electron promotions from the σ(SiSi) type HOMO, each into one of the two virtual orbitals that compete for the status of the lowest unoccupied molecular orbital (LUMO). One of them is of the σ*(SiSi) type and the strongly allowed excitation into it produces the 1*B* σσ* state. The other is of the π*(SiC) type and the very weakly allowed excitation into it produces the 2*A* σπ* state.

The oscillator strength *f* of the transition into the 1*B* state is proportional to *n*. The calculations reproduce this trend well but the absolute values of *f* are too large and the excitation

energies are a little too high. They drop almost linearly with $1/n$, with a slope of $[dE(1B)/d(1/n)]_{n=\infty} = 72.3\times10^3$ cm^{-1}, and extrapolate to a limit of 27 500 cm^{-1} at infinite chain length and $\omega = 180°$.

The 2*A* excited state carries negligible oscillator strength. Its energy drops only slightly less linearly with increasing *n*, but with only about half the slope, $[dE(2A)/d(1/n)]_{n=\infty} = 42.4\times10^3$ cm^{-1}. The 2*A* state lies below 1*B* in the shortest oligosilanes, but in all permethylated oligosilanes with more than five or six Si atoms, it lies above 1*B*. As noted above, experimental evidence for the presence of the 2*A* state is available in a trisilane, *n*-tetrasilanes and *n*-hexasilanes.

Other transitions of negligible intensity follow at higher energies. The energy of the 2*B* and 3*A* states drops rapidly with increasing *n*, and the 2*A* and 3*A* states touch near $n = 12$. At smaller values of *n*, the 2*A* state is σπ* (excitation from HOMO to π*) and the 3*A* state is σσ* (excitation from HOMO−1 to σ*). At larger values of *n*, the 2*A* state is σσ* (HOMO−1 to σ*) and the 3*A* state is well approximated as σπ* (HOMO to π*). Finally, the 2*B* state, always well separated in energy from the 1*B* state, is of σπ* nature. Its energy also drops rapidly with increasing *n* and it is possible that in very long chains it lies below the 3*A* state.

Tight-Helix Oligosilanes. Steric hindrance prevents the construction of the other natural limit for the oligosilane chromophore, with a dihedral angle $\omega = 0°$. This limit is therefore purely hypothetical and we cannot use TD DFT theory to calculate its properties, although we still can examine them in simple models such as Ladder C and Ladder H.

Using all-*gauche*-$Si_{12}Me_{26}$ as an example, Figure 8B shows the form of the molecular orbitals involved in low-energy transitions and demonstrates how dramatically they differ from the analogous orbitals in the all-*anti*-$Si_{12}Me_{26}$ conformer (Figure 8A). The contrast is even more easily seen in the symbolic representation of the MOs of $Si_{16}Me_{34}$ in Figure 9. The segmentation of the orbitals in the all-gauche case is very different from the even delocalization in the all-anti case and makes it

understandable why the energy of the HOMO changes so little with chain length in the former while it increases rapidly with increasing chain length in the latter.

At ω = 55°, the σσ* character has mostly disappeared even from the 2*B* state and moved to states that are still higher in energy. It would thus appear that in the unreachable limit of ω = 0°, the σσ* excitation energy would be very high. The four lowest energy excited states are primarily σπ*. Transition oscillator strength follows the nature of the excited state, and as σ to σ* excitation character disappears from the 1*B* excitation, so does the intensity. At dihedral angles smaller than 90°, all four lowest transitions are predicted to carry nearly no oscillator strength at all.

These changes in the nature and intensity of electronic excitation are accompanied by similarly dramatic changes in transition energy. The $[dE(1B)/d(1/n)]_{n=\infty}$ slope is 13.8×10^3 cm^{-1} at 55°. The slope for the 2*B* state (31.2×10^3 cm^{-1}) is about twice the slope for the 2*A* state (16.6×10^3 cm^{-1}).

2.3.2. Simple Hückel Models for Loose and Tight Helices

It is reasonable to expect the huge difference between the properties of loose and tight helical conformations of oligosilanes to be a fundamental feature, present even in the simplest models of σ delocalization. We next examine models that operate at the Hückel level: the Ladder H that considers all four valence orbitals on the silicon atom as well as orbitals on substituents that are attached to the silicon backbone, and the even simpler Ladder C that considers only the two valence orbitals on each silicon atom that are used to form the oligosilane backbone.

Figure 10 compares the HF and KS HOMO energies with those obtained with the Ladder H and C results using standard parameters and demonstrates that all four methods predict qualitatively and even semiquantitatively the same dependence of the HOMO energy on *n* and ω. Energies of other occupied MOs calculated with the Ladder H model also are in a good agreement with HF orbital energies, as are the energies of occupied σ MOs obtained with the Ladder C model. The largest discrepancies, about 0.3 eV, are found for longer chains in loose conformations. Figure 9 shows that the orbital shapes and nodal properties, too, are very similar in the DFT and in the Ladder model calculations, although the size and distribution of the islands observed in the HOMO at small values of ω are not identical (the KS HOMO is of a different symmetry than those in the Ladder models, and this is due to a different MO energy ordering within a tightly packed group of MOs). The general agreement is not surprising, since the parameters in the Ladder models were chosen by fitting HF energies of occupied MOs,[5] albeit over a limited range of conformations (the KS orbital energies are 2.0 to 3.0 eV higher than HF energies and have been shifted up by 2.3 eV in Figure 10). The results shown in Figures 9 and 10 justify the use of the simple Ladder models in our effort to find an intuitive explanation of the origin of the strong conformational effects on σ delocalization in oligosilanes.

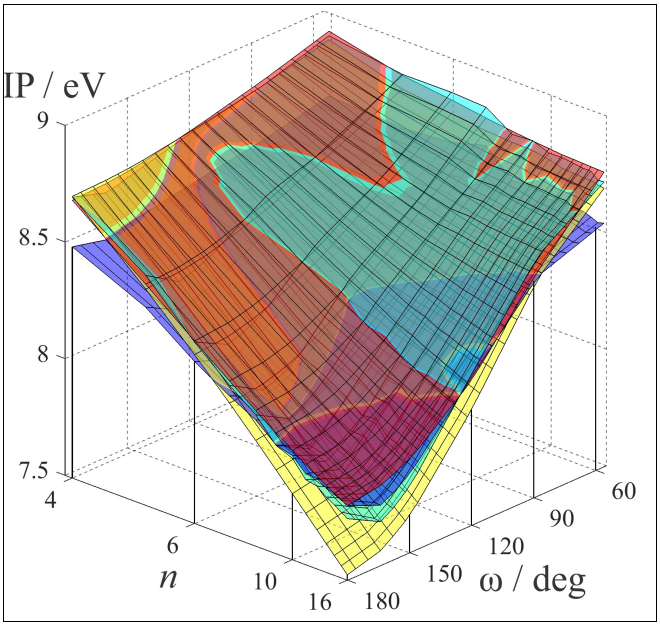


Figure 10. The ionization potential of all-[ω]-**1[*n*]** (*n* = 4 - 16) calculated in the Koopmans approximation with: Ladder C (red), Ladder H (yellow), HF/TZ (green), and DFT/TZ (blue, shifted up by 2.3 eV).

The partition ratio values p_{HOMO} obtained from Ladder C calculations (Figure 11) provide a quantitative measure of σ delocalization and confirm the qualitative conclusions reached so far. Its high value in the ω = 180° limit marks a high degree of σ delocalization, and it remains high down to about ~90°. At smaller dihedral angles, it drops precipitously. It is interesting to note its quasiperiodic dependence on *n* in the ω = 0° limit, which reflects the growth in the number of high amplitude islands as the chain grows longer.

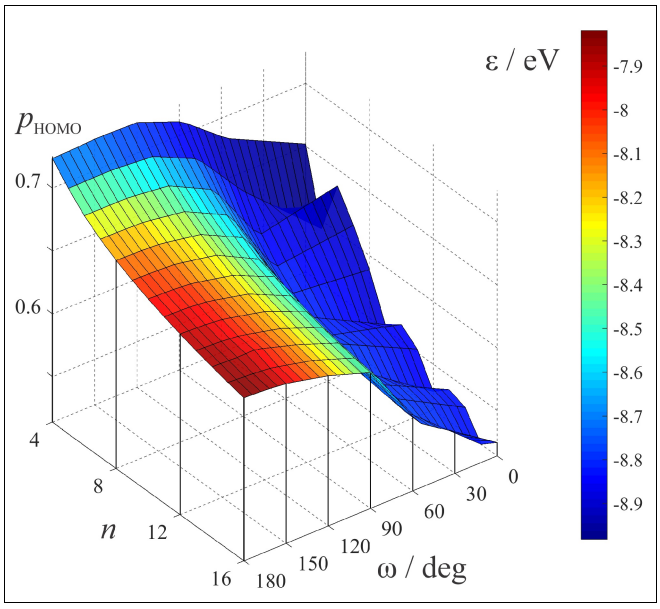


Figure 11. The HOMO partition ratio of all-[ω]-**1[*n*]** (*n* = 4 - 16) in Ladder C model (color indicates HOMO energy).

The qualitative similarity of the HF, KS, Ladder H, and Ladder C HOMO orbital energy behavior as a function of *n* and ω is illustrated in more detail in Figure 12. In the loose helix limit, the HOMO energy is sensitive to chain length. In the tight helix limit, all four methods agree that the HOMO energy changes only slightly as the chain length increases. In the region ω = 90 - 120° the two limiting cases meld into each other, with the loose helix characteristics dominant. The tight helix behavior does not dominate fully until ω is reduced to about 60°. Even the largest qualitative difference between the conclusions drawn from the Ladder models and those drawn from the DFT and HF methods is only tiny. In the former, for any *n* the maximum of the HOMO energy is at the all-anti conformation (ω = 180°) whereas in the latter, it is at the all-transoid conformation (ω = 163°).

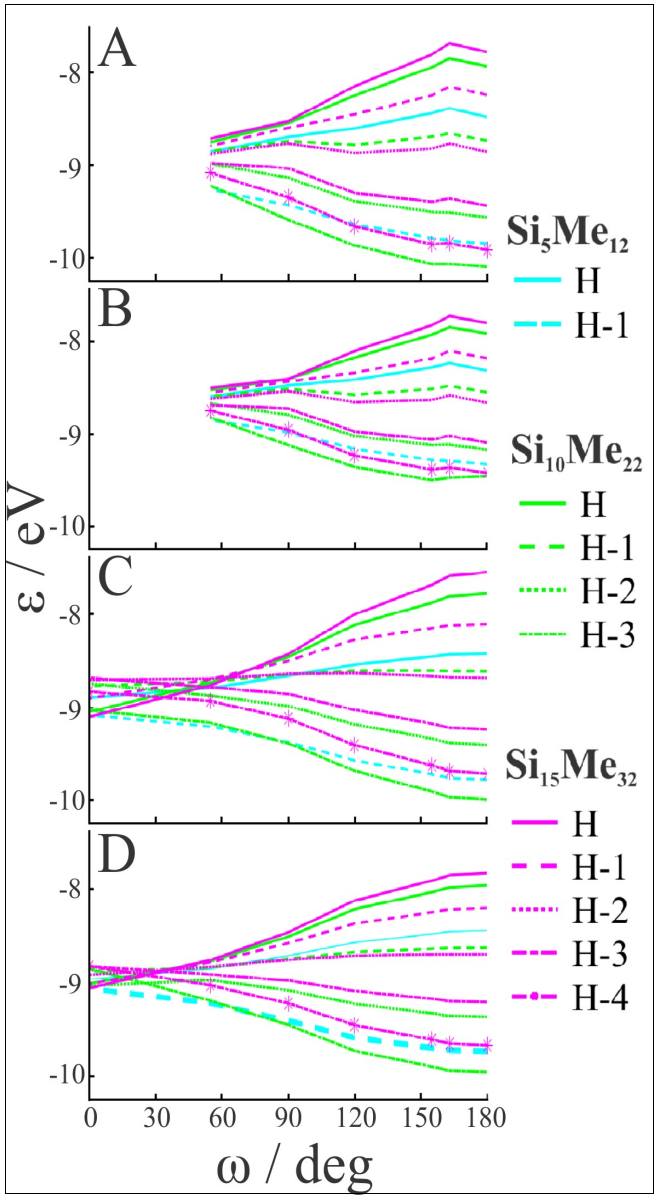


Figure 12. Energies of several highest occupied MOs in Si_5Me_{12}, $Si_{10}Me_{22}$, and $Si_{15}Me_{32}$ as a function of ω, calculated with HF/TZ (A), DFT/TZ (B), Ladder H (C) , and Ladder C (D) methods. H stands for HOMO. A constant (-2.3 eV) was added to DFT/TZ orbital energies.

Figure 12 also shows that the similarity of the trends displayed by DFT calculations and those obtained with the Ladder methods extends to lower energy orbitals. All four computational methods show that the width of the band of occupied σ orbitals increases as the chain length grows, hardly a surprise, but they also show that it does so very much more in the loose helix than in the tight helix limit. In the Ladder model calculations, where the limit ω = 0° can be reached, the orbital energies actually cross at about 30 - 40° and then invert their order. The conclusions reached are entirely compatible with those reached from DFT excitation energies (Figures 5 and 7), HOMO shapes (Figures 8 and 9) and energies (Figure 10), and from the plot of p_{HOMO} in Figure 11: in loose helices σ delocalization is strong and chain length matters, whereas in tight helices σ delocalization is weak or absent and chain length hardly matters at all.

Although the Ladder models can thus be used to analyze the effects of σ delocalization in terms of HOMO energies, they cannot be used for predictions of energies of virtual orbitals and of excitation energies, since they do not perform well for the relative energies of σ* and π* unoccupied orbitals and the Hückel approximation of equating excitation energies to orbital energy differences alone is inadequate. In the Ladder C model, σπ* transitions are absent altogether. Ladder H attributes much lower energies to σ* than to π* unoccupied orbitals, all predicted low-energy transitions are pure σσ*, and in this important region all σπ* transitions are missing. This may be due to the absence of electron repulsion terms in the expression that relates excitation energies to orbital energy differences, and could perhaps be corrected by an elaboration of the Ladder H model beyond the Hückel level. At this time we prefer to simply acknowledge that the current version of this model is incapable of describing low-lying excited states of linear oligosilanes properly, and we shall confine our discussion to the properties of the HOMO.

2.3.3. An intuitive rationalization of the contrast between loose and tight helices

Why is the nature of the HOMO so different in the loose and the tight helices, making the former strongly σ-delocalized and the latter essentially σ-localized? In the following, we provide an intuitive answer at the level of the Ladder C model, and use the similarity of the results of the several approximations used here to claim the answer is valid generally, at least within a certain range of relative strengths of geminal and vicinal interactions (σ conjugation and σ hyperconjugation).

We start by recognizing that the description of a long linear *n*-Si_nMe_{2n+2} chain in which the absolute values |ω| of all backbone dihedral angles are the same requires only three values of resonance (hopping) integrals: β_p (primary), β_g (geminal), and $\beta_v(\omega)$ (vicinal). Actually, with β_p as the energy unit, the model is fully described by the ratios $g = \beta_g/\beta_p$ and $v(\omega) = \beta_v(\omega)/\beta_p$, which describe the relative importance of σ conjugation and σ hyperconjugation, and strongly depend on the choice on the backbone chemical element, the valence angle within the chain, and the length of the backbone bond. In Chapter III, we consider the range of the $[g,v(\omega)]$ space within which the current conclusions hold, but presently we merely accept the values $g = 0.31$ and $v(\omega)$ ranging from -0.23 at ω = 180° to 0.17 at ω = 0° that have been determined for permethylated oligosilanes by fitting to HF MO energies.[5] Thus, the results of the present analysis are valid for standard SiSi bond lengths of ~2.36 Å and SiSiSi valence angles of 114°, typical of permethylated oligosilanes.

We first obtain inspiration from a plot of Ladder C p_i values for all σ(SiSi) MOs of $Si_{16}Me_{34}$ as a function of ω (Figure 13B; the explicit form of all these MOs is shown in Figures 13A and 13C). In the first approximation, the plot has the shape of a tilted saddle, with the highest values (the most σ delocalization) for the highest few energy MOs (and especially, the HOMO) in loose helices and the lowest few energy MOs in tight helices. Low values (the least σ delocalization) are found for the few lowest energy MOs in loose helices and the few highest energy MOs, including the HOMO, in tight helices. This is as expected, since the degree of σ delocalization in the chain is judged by the properties of the HOMO. Figure 13 shows that the internal structure of the least stable MO in loose helices is similar to that of a much more stable one in tight helices and that the most stable MO in tight helices resembles a much less stable one in loose helices. It thus appears that the order of the MOs is approximately inverted upon going from one to the other conformational limit. Such an inversion would be expected if the relative signs of resonance integrals along the chain differed in

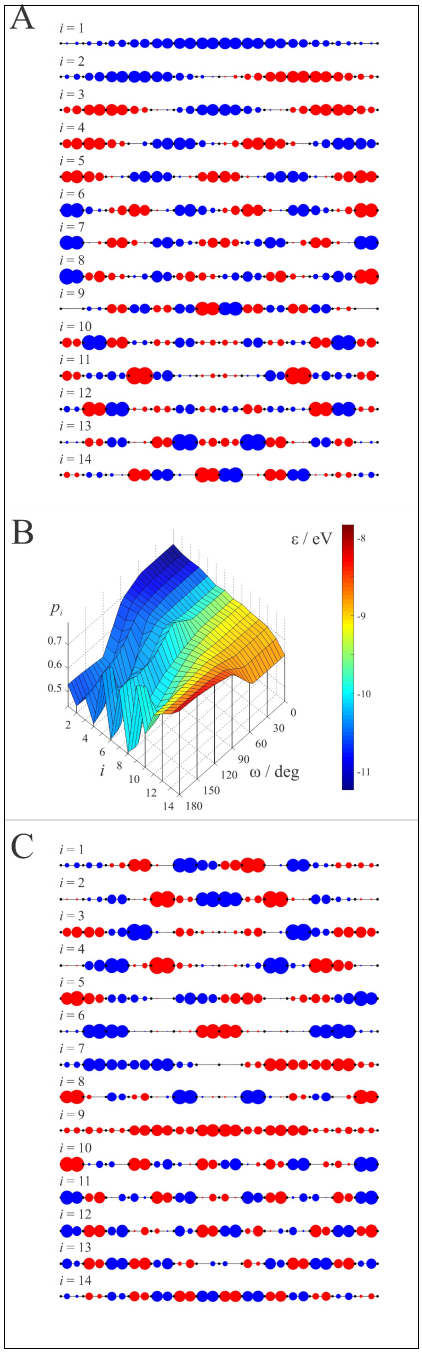


Figure 13. All-[ω]-$Si_{15}Me_{32}$ in the Ladder C model: Symbolic representation of the 15 σ(SiSi) MOs at ω = 0° (A) and 180° (C), numbered from the most to the least bonding, and their partition ratio as a function of ω (B, color indicates MO energy).

the two limiting conformations ω = 180° and ω = 0°. The only ones that change sign are $\beta_v(\omega)$, characterized by the ratio $v(\omega) = \beta_v(\omega)/\beta_p$. This observation suggests a two-step analysis in which β_g is ignored at first, as outlined in the following.

In the first step, we construct an MO energy diagram assuming $g = 0$. In that case, the oligosilane chain separates into two mutually non-interacting linear chains of NHOs containing σ bonds indicated in Figure 14 in violet and green solid lines, respectively. The much weaker vicinal interactions within each chain, also colored violet and green, are indicated as dotted lines. When n is odd, the two chains are identical and each contains $(n - 1)/2$ σ(SiSi) bonds. When n is even, one of the chains contains $n/2$ and the other contains $(n/2) - 1$ σ(siSi) bonds. The chains are assumed to be long enough for end effects on orbital coefficients and node positions to be negligible and for the difference between $n/2$ and $(n/2) - 1$ to be negligible as well. Each of the two subchains is topologically equivalent to a linear polyene with strongly alternating interaction integrals β_p and β_v. The resulting MO energies are all doubly degenerate (exactly when n is odd and approximately when n is even) and for each value of ω they are located within two identical vertical bands in the energy diagram for the bonding σ MOs.

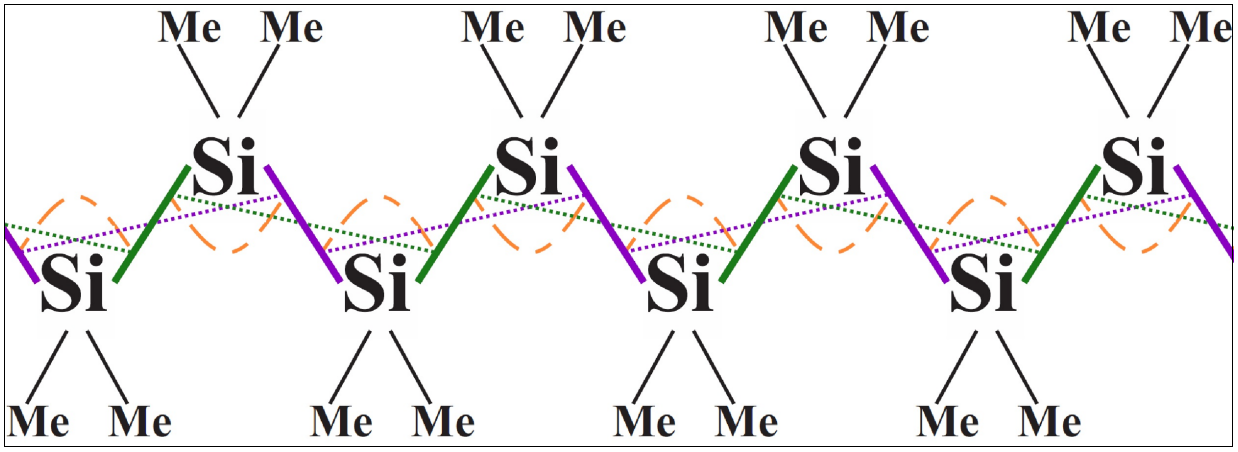
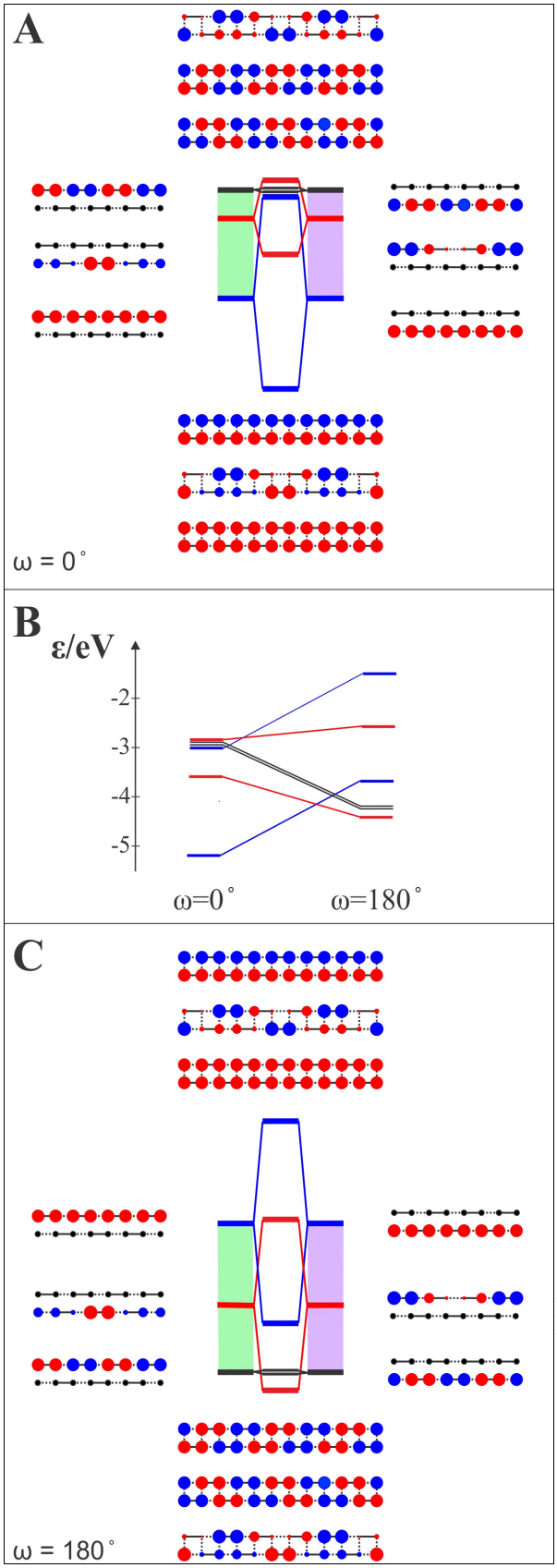


Figure 14. Resonance integrals in a permethylated oligosilane chain: primary (full), vicinal (dotted), and geminal (dashed) interactions. The green and violet colors show the division into two equivalent mutually non-interacting linearly conjugated side pieces in the absence of geminal interactions across the ladder rungs (orange).

In Figure 15 these bands are shown in violet and green in both limits, $\omega = 180°$ and $\omega = 0°$. In each case, only three energy levels in each chain are shown explicitly: the most stable one at the bottom of the band, the least stable one at the top of the band, and one of the intermediate levels. In Figure 16, we show the Ladder C p_i values for all the MOs in a color code.

The nodal structures of the least stable and the most stable MO within each colored band are shown symbolically, in Figure 15A for the all-syn case $\omega = 0°$ and in Figure 15C for the all-anti case $\omega = 180°$. The MO coefficients are nearly uniform over each non-interacting chain. Their magnitudes and signs at the two NHOs located on each silicon are indicated in color and are shown above each other at the ends of rungs in a long ladder, connected by side pieces in which the primary and the vicinal interactions alternate. The upper side piece contains all the NHOs forming the green set of SiSi bonds in Figure 14 and the lower piece contains all the NHOs that are responsible for the violet set of SiSi bonds. At the moment, there is no interaction across the rungs that connect the two side-pieces. As expected for occupied σ bond orbitals, in both the all-anti and the all-syn limit, the



signs of the MO coefficients at the two ends of every primary interaction within each oligosilane ladder side piece are equal.

However, because of the difference in the sign of β_v at $\omega = 180°$ and $\omega = 0°$, the energy order of the MOs within each colored band is opposite in the two conformations. In the all-anti conformation, $\beta_v > 0$, the least stable MO is the one that has no nodes at all cutting the ladder, and the most stable MO is the one that has a node across each vicinal interaction. In the all-syn

Figure 15. Ladder C MO energy diagrams for (A) all-syn ($\omega = 0°$) and (C) all-anti ($\omega = 180°$) conformations of an oligosilane. Orbital energies of two equivalent (odd *n*) or nearly equivalent (even *n*) mutually non-interacting linear chains (green and violet in Figure 8, $v = 0.17$ at all-syn and $v = -0.23$ at all-anti, $g = 0$) on the left (green stack) and right (violet stack). In the middle (white stack), after geminal interactions ($g = 0.31$) are introduced to first order. Schematic orbital structure before interaction is shown on the sides of the diagram, and after interaction, on the top and bottom (the two NHOs on each Si atom are placed above each other, full lines represent primary and dotted lines vicinal interactions). The top to bottom ordering of the orbital sketches after interaction (center) follows the ordering of the orbital energy levels. (B) An all-syn to all-anti correlation diagram showing the energies of selected MOs for oligosilane chain. Dashed lines connect orbitals with identical nodal properties.

conformation, $\beta_v < 0$, and the situation is reversed. Unlike the MOs located at the top or bottom of the colored bands, the MOs whose energy is located inside the colored bands have an intermediate number of nodes and consist of groups of NHOs that carry large amplitudes separated by regions of almost no amplitude, similar to what is seen in Figure 13AC and on the right in Figure 9. One such intermediate energy orbital in each stack is shown explicitly. The p_i values indicated by color in Figure 16 for the same stacks of orbital levels of the subchains make the delocalized nature of the least and the most stable orbitals in each stack and the more localized nature of the orbitals located at intermediate energies clear.

So far, the least bonding (HOMO) and the most bonding among the MOs in the two identical colored stacks of MO levels are both perfectly delocalized and

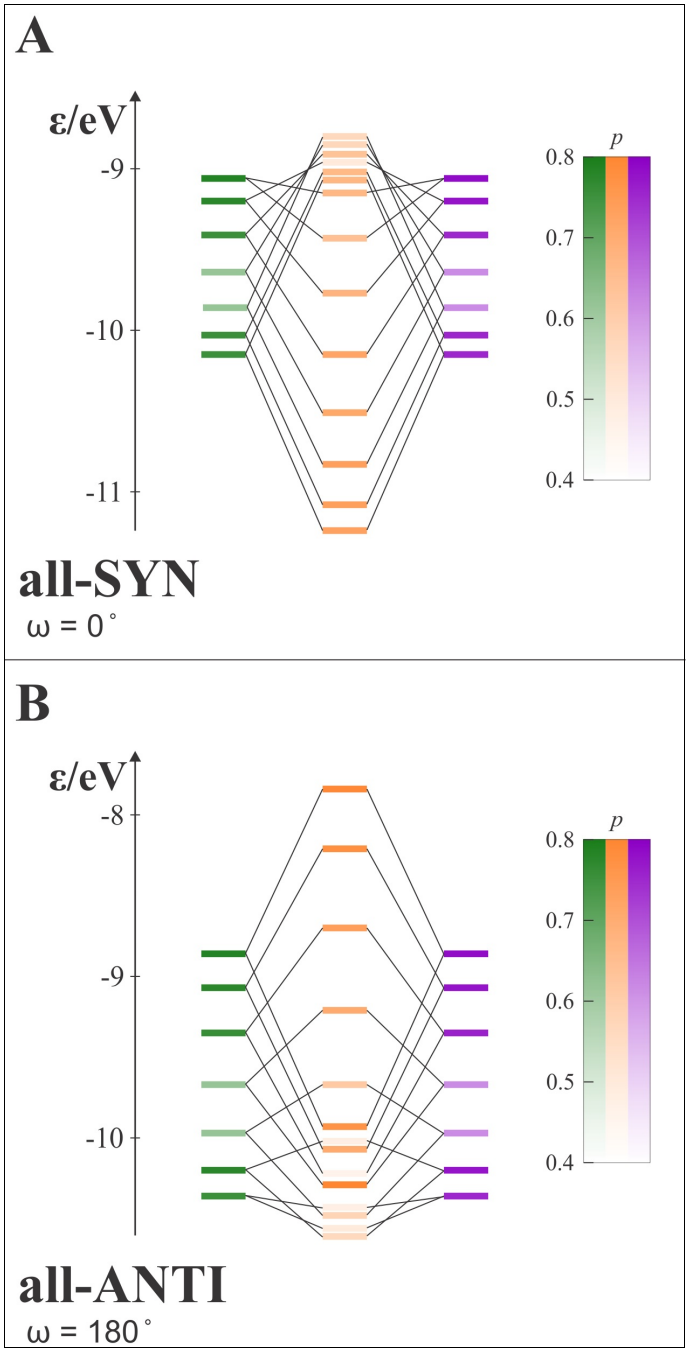


Figure 16. Energy diagrams for (A) all-syn and (B) all-anti conformations of $Si_{15}Me_{32}$ in the full Ladder C model: Left and right, MO energies of the green and violet NHO chains (cf. Figure 8) before they are allowed to interact ($g = 0$). Center (orange), MO energies after geminal interactions are introduced ($g \neq 0$). Color shade indicates the partition ratio.

ready to respond to further chain extension, and there is no reason to expect the all-anti conformer to σ delocalize and the all-syn conformer not to do so. This will change in the next step, where we introduce the geminal interactions β_g across each of the rungs of the ladder to produce the complete Ladder C Hamiltonian. These cause a formation of in-phase and out-of-phase combinations of degenerate (or nearly degenerate, if *n* is even) levels from the two colored stacks in Figures 15A and 15C, one representing the energies of MOs from the violet side-piece and the other those from the green side-piece. One of these combinations is stabilized and the other is destabilized, and the results are shown in the central column. In the first approximation, the formation of the sums and differences will not affect the relative p_i values over the now doubled number of sites *m*. However, the splitting changes orbital energies from their initial values in each subchain, possibly quite significantly, and introduces the irregularities that appear in the loose helix limit in Figure 13.

In the first approximation, the magnitude of each splitting is dominated by the match of the nodal properties of the MOs in the two colored columns as the summation of interactions over all rungs (Si atoms) in the molecule is performed (Figure 15). The least stable MO in the all-anti case and the most stable MO in the all-syn case, which contain no nodes, are matched perfectly and give the largest splitting. The most stable MO in the all-anti case and the least stable MO in the all-syn case are perfectly mismatched, the contributions from adjacent rungs cancel, and the summation over all rungs yields zero. As a result, for these levels the contributions from the violet and the green side-pieces will still mix even in first order, but their energies will not change at all. For MOs whose energies lie between the two extremes the splitting will be of intermediate size, and one such example is shown for both the all-anti and the all-syn case. In Figure 16, we show the MO energies that result from the full diagonalization and it is seen that the pattern corresponds to that obtained

in the first-order approximation in Figure 15, but there are differences in the level positions because now mixing with antibonding MOs is taken into account.

What, then, will the HOMO look like? In the all-anti case, Figure 15C leaves no doubt: it will be the destabilized combination of the levels from the violet and green columns, just as anticipated from all four types of calculation performed here. This conformer is σ-delocalized and has a high p_{HOMO} value. Inspection of its uniformly delocalized HOMO makes it clear that further extension of the oligosilane chain will lead to additional destabilization of the HOMO. In the all-syn case, the situation is less clear. The HOMO level could be the doubly degenerate combination of the least stable levels from the violet and green stacks, in which case it would also be fully σ-delocalized, or it could perhaps happen that the interaction of one of the lower-lying degenerate levels, one from the violet and one from the green side piece, will be strong enough to push the resulting destabilized combination even higher and cause it to become the HOMO. This combination will then possess some intermediate number of nodes and will look like the MOs on the right-hand side of Figure 10B, which contain several mutually almost non-communicating regions of large amplitude. Just how many nodes there will be and how large the regions will be is likely to depend strongly on the details of the situation and cannot be stated in general. An extension of the chain will then merely add one or more nearly non-interacting regions and this conformer will be σ-localized.

Which of the situations occurs will depend on the values of $v(\omega)$ and g and the ranges of values in which one or the other outcome prevails will be addressed in Chapter III in a more quantitative fashion in the infinite chain limit. The use of standard Ladder C parameters for oligosilanes predicts that the all-syn limit will be σ-localized, as indicated in Figures 13, 15 and 16.

The orbital level correlation between the ω = 0° and 180° is shown in Figure 15B and provides a simple explanation of the main features of Figure 12.

The origin of the difference in σ electron delocalization between the all-anti and all-syn limits in permethylated oligosilanes is now clear. In general, the relative importance of geminal and vicinal interactions (σ conjugation and σ hyperconjugation) will be critical in determining the outcome. Note that only the absolute value |ω| enters into the arguments and the sense of the local helicity does not.

2.4. Discussion

All-*t* and All-[*ca*] Conformers. The experimental results for these conformers validate the TD-DFT B3LYP/TZ method of calculation of the dependence of the singlet excitation energies on chain length for two extreme cases: strong dependence on chain length in the all-*t* conformer series (strong σ delocalization), and independence of chain length in the all-[*ca*] conformer series (no σ delocalization). Figure 4 shows that the computations reproduce the behavior of the energy and the intensity of the first observed absorption maximum in samples with random sense of helicity quite well. It is also known that they perform well for the weak transitions in Si_3Me_8[91] and a few tetrasilanes[4,91,94] and hexasilanes,[110] and it is reasonable to assume that the TD-DFT B3LYP/TZ level of computation also describes the regular helical conformers correctly.

Regular Helical Conformers. With the exception of the all-*t* conformers (ω = 163°), where the agreement with measurements on conformers with a random helical sense (|ω| = 163°) is excellent (Figure 4), the results shown in Figures 5 and 7 represent predictions. At low energies, they are likely to be quite dependable, but above 50 000 cm^{-1} Rydberg states are likely to intervene

and the results cannot be trusted to nearly the same degree. Therefore, we focus our discussion on the 1*B*, 2*A*, 3*A*, and 2*B* excited states. The course of the energies of the 2*B* and 3*A* states as a function of *n* shows irregularities that appear to be due to avoided crossings with higher energy states, but we do not discuss these in detail since as stated we suspect that in this energy range the results are not dependable.

The conformational dependence of the predicted spectra of regular helical conformers thus is vaguely reminiscent of the response of oligosilanes to chain length doubling, discussed earlier in terms of the Ladder C model.[6] A doubling of the number of SiSi bonds causes almost the same red shift of the σσ* transition as long as the two newly created internal dihedral angles remain in the range 180 - 120° (σ-delocalized conformations). This is followed by an abrupt change to a much smaller or no red shift as the angles become smaller (σ-localized conformations).

The Difference between the Loose-Helix and Tight-Helix Oligosilane Chromophores. In common parlance, the loose-helix oligosilanes are σ-delocalized ("σ-conjugated") and the tight-helix oligosilanes are not. This puzzling experimentally observed behavior is faithfully predicted by the present calculations and its origin is now qualitatively clear from a consideration of the all-anti and all-syn limits for a helical chain. The key to the simple understanding is provided by the consideration of an intermediate approximation in which geminal interactions are neglected. The ladder arrangement of approximate sp^3 hybrids in the oligosilane chain is then split into two non-interacting side pieces that are topologically equivalent to two polyenes with strongly alternating bond lengths. If *n* is odd, each side piece contains half of the Si-Si bonds, and if *n* is even, one side piece is one bond longer. A change of sign of the vicinal resonance integral β_v that is induced by going from loose to tight helices inverts the energy order of the MOs in each side piece. As a result, when the geminal interaction is finally introduced, the MOs that combine to produce the HOMO are

very different in the two types of helices. In loose helices ($\beta_v > 0$), there is no doubt that the HOMO will be fully σ delocalized. In tight helices ($\beta_v < 0$), depending on the values of *v* and *g* that characterize the strengths of geminal (σ conjugation) and vicinal (σ hyperconjugation) interactions, the HOMO could have a node at every other Si atom and still be fully delocalized, or it could have an intermediate number of nodes and be fragmented into a series of mutually nearly non-interacting islands, producing a σ-localized system. For oligosilanes, the values of *v* and *g* are such that the latter situation obtains.

2.5. Conclusions

The present work has led to two conclusions: (i) The B3LYP/6-311G**//MP2/6-311G** TD-DFT method reproduces correctly both the strong chain-length dependence of the first singlet excitation energy in peralkylated all-*t* oligosilanes and its near chain-length independence in peralkylated all-[*ca*] oligosilanes. In both types of measured samples, the sense of local helicity is random. This method of calculation should be useful for computing vertical excitation energies of various conformers of peralkylated oligosilanes in general. (ii) The origin of the predicted strong dependence of the excitation energies and ionization potentials of peralkylated regular helical oligosilanes on the skeletal dihedral angle ω is easy to understand in intuitive terms by consideration of a correlation diagram between two limiting chromophores, the σ-delocalized real all-*a* (ω = 180°) and the σ-localized purely hypothetical all-*c* (ω = 0°). The key to the simple description is the consideration of the interaction of two linearly conjugated structures, each built from half of the σ(SiSi) bonds present, when σ conjugation (geminal interactions) is introduced.

Chapter III

Effect of Conformation on Electron Localization and Delocalization in Helical Chains $(XMe_2)_\infty$, X = Ge, Sn, and Pb

3.1. Introduction

The success of the Ladder C model in explaining the conformational dependence of electron delocalization in oligosilanes motivates further study. Properties of oligo- and polysilanes show similar conformational dependence,[111] prompting the question how the effects of electron (de)localization in molecules translate into properties of infinite, inherently delocalized systems and how these effects can be quantified. Known resemblance of conformation-dependent properties in oligosilanes and oligogermanes provokes us to ask if similarities and differences in the electronic behavior of electron behavior in catenanes of various elements of group 14 can be understood in simple terms.[112] Finally, one must ask how good the insights from a simple model are and if they correspond to reality.

Present chapter provides an answer to these questions. The connection between finite and infinite systems is explored through study of conformational effects on the band structure of helical polymers. We find that the band structure of $(XMe)_2$, where X = Si, Ge, Sn, Pb, changes significantly with the conformation, leading to an alteration of properties. The band structure changes correlate well with the electronic structure changes in finite molecules, such as the energy and form of the HOMO. Comparison of electronic structures belonging to helices with different backbone atom offers an insight into noted similarities and differences between analogues of

oligsilanes. The DFT calculations match well with Ladder C predictions, confirming that simple insights proposed at Ladder C level are true.

Although the Ladder C model offers a simple and intuitive explanation of some properties of σ delocalized systems, its power is limited by assumption of the model. Alkanes are not part of present study because π-type orbitals, which are not present in the Ladder C model, have significant effect on the electron delocalization in these compounds. Similarly, the Ladder C model cannot be used to study excited states, where π* orbitals are important, which is why the study is exclusively focused on the ground state properties. Nevertheless, we believe that main characteristics of electron delocalization in σ-bonded systems are well captured already at the Ladder C level, and that additional studies at Ladder H level could just increase our understanding of the details of specific systems.

3.2. Methods

3.2.1. Parametrization of Ladder C Model

Ladder C parameters for X = Si were determined previously by fitting of energies of occupied molecular orbitals to those obtained from Hartree-Fock (HF) calculations for a series of short chains at a variety of MP2-optimized conformations.[5] Similar procedure has been used in the present work for X = Ge, Sn, and Pb. In the case of oligosilanes, the MP2 method was used as opposed to DFT because, at the time, it provided dihedral angles $\omega_{SiSiSiSi}$ that were in better agreement with experiment. Chemical similarity between oligosilanes and oligogermanes motivated us to use the MP2 method to obtain optimized geometries used to find Ge parameters. However, we have decided

that the potential differences between DFT and MP2 geometries are not significant enough in the cases of Sn and Pb, and chosen to used DFT for geometry optimizations of oligostannanes and oligoplumbanes. This assumption was confirmed by comparing experimental and calculated equilibrium bond lengths and bond angles.[113]

RI-MP2 geometry optimization was performed on 27 conformers of Ge_nMe_{2n+2}, n = 2 - 7, using Turbomole software.[114] The basis set for Ge was 6-311G*, for C 6-31G*, and for H 6-31. All but nine conformers were optimized to minima on the potential energy surface (PES). The nine that do not correspond to minima resulted from constrained geometry optimizations with frozen GeGeGeGe dihedral angles and optimization of the remaining degrees of freedom. At the 27 geometries, HF calculations with NBO analysis were performed to obtain MO energies, using Gaussian 09 software.[115] Geometry optimizations with RI-PBE0/def2-TZVP/J and (RI) ZORA correction were done for 24 conformers of Sn_nMe_{2n+2}, n = 2 - 7, and 17 conformers of Pb_nMe_{2n+2}, n = 2 - 6, using Orca 3.0 and Orca 4.0 software.[116, 117] All conformers were optimized to the closest local minimum. MO energies and NBO analysis were performed at the HF/def2-TZVP level with RI ZORA correction, using Orca 4.0 and NBO6 software.[118]

The program previously used to obtain Ladder C parameters for silicon was used to find the five adjustable parameters for each of Ge, Sn, and Pb.[5] It fits Ladder C to HF MO energies using the Powell minimization procedure.[119] The error function was the square of the sum of root mean square (RMS) deviations of the Ladder C and HF orbital energies. The fitting started by calculating the overlaps between the HF orbitals, expressed in the valence part of Weinhold's natural hybrid orbital (NHO) basis,[49] and the Ladder C orbitals calculated with an initial guess for parameters. Once the orbitals were matched, the differences in orbital energies were decreased by parameter optimization. The optimized parameter values for Si were used as the initial guess for Ge, those

optimized for Ge were used as the initial guess for Sn, and the optimized parameters for Sn were used as the initial guess for Pb. The error function is irregular in the space of Ladder C parameters and contains many local minima of similar depth. Some of these appeared unphysical and were disregarded, but many ill-defined shallow minima differing only slightly in parameter values remained. These parameter values were averaged and used as a starting point for a new minimization. Finally, overlaps were recalculated using new parameters. They are large for the higher energy occupied MOs, well described as σ bonding, and smaller for lower energy occupied orbitals, which have mixed σ-π character in the HF description.

It was found that the energetically upper half of Ladder C occupied MOs and the highest occupied HF MOs are always in the same order. In most cases, the order of the lower half of the Ladder C occupied MOs was the same as the order of HF orbitals, too, but there were some exceptions in case of the MOs that have a significant π component, which cannot be described by the Ladder C model. The difference in ordering of the lower energy occupied Ladder C and HF orbitals was largest for Ge. Here, the fitting was done in two steps, first for those conformers in which all Ladder C orbitals were in the same order as HF orbitals, and then for all conformers. In the other cases, the fitting was done in a single step, using all conformers.

By basing the parameterization on results obtained for geometries of local ground state minima, albeit for a wide range of dihedral angles ω, we consciously bias the model toward optimal description of conformers of XMe_{2n+2} that are actually likely to be present at ambient temperatures and below. This is desirable for the free chains, but we recognize that often attempts are made to force the chains to adopt other conformations by structural modifications such as introduction of cycle-forming saturated structures,[120] and that these interventions may result in unintended changes in valence angles and possibly even in XX bond lengths. Even though Ladder C model could be

parameterized to allow changes in valence angles and bond lengths, additional parameterization would not deepen our understanding of the behavior of linear chains, but only give slightly better quantitative results. Finally, in chains containing more than one type of skeletal atom, one would need to introduce additional interaction integrals $\beta_p(XY)$ and $\beta_v(\omega,XY)$, but we will not consider such cases here.

3.2.2. DFT calculations on infinite helices

Periodic calculations were carried out using CRYSTAL17 software,[121] at DFT level, using PBE0 functional for exchange and correlation.[122, 123] Calculations for $(SiMe_2)_\infty$ and $(GeMe_2)_\infty$ were done using POB-TZVP basis set on all atoms.[124] In $(SnMe_2)_\infty$ and $(PbMe_2)_\infty$ calculations POB-TZVP basis set was used on C and H atoms, while small core pseudo-potentials with 28 (ECP28MDF) and 60 (ECP60MDF) core electrons and cc-PVTZ-PP basis set for valence electrons were used on Sn and Pb, respectively.[125,126,127]

Molecular parameters, such as bond lengths, valence angles, and torsion angles were optimized within requirements of a line group of a helix.[42] Line groups are characterized by two integers: N_1, a number of roto-translational units in a pitch of a helix, and N_2, which determines number of full turns needed to form a translational unit cell. This kind of geometry optimization leads to geometries that represent either a minimum or a maximum on the potential energy surface (PES). The structures that were kept were either minima or maxima that have non-zero frequencies that correspond only to vibrations of the backbone, analogous to the constrained optimizations in finite molecules. Different line groups correspond to different conformers on the same compound, as dihedral angle is a molecular parameter that changes the most between line groups. Band

structure calculations were carried out in the first Brillouin zone (FBZ). DFT calculations used translationally invariant unit cell containing all atoms in a full pitch of a helix (N_1 XMe_2 groups). Effective hole and electron mass were calculated using Effective mass calculator (EMS) code.[128]

3.3. Results

3.3.1. Ladder C parameters

The final optimized parameters are listed in Table 1 and are expected to work best for equilibrium geometries. The similarity of Pauling electronegativities (1.90 for Si, 2.01 for Ge, 1.96 for Sn, and 2.33 for Pb)[129] of all four elements is reflected in the values of the Coulomb integral α. As the atomic number increases, XX bonds weaken, and absolute value of the negative integral β_p decreases. In the current version of the Ladder C model, the integrals are not affected by changes in valence angles and the percentage of *s* and *p* orbitals contained in the hybrid.[130] Typical lengths of the XX bonds are 2.36 Å for Si, 2.43 Å for Ge, 2.80 Å for Sn, and Å for 2.92 Å for Pb. The optimized valence angles are almost the same for all elements, with typical value 113 ± 5° for all elements. The same is true for the *ns* - *np* energy differences between the AOs (6.71, 7.88, 6.91, and 8.56 eV for Si, Ge, Sn, and Pb, respectively).[131] It is thus not surprising that the negative β_g values are quite similar for all four elements. Vicinal integrals are also very similar throughout the series, positive at the anti and negative at the syn geometry. The favored skeletal dihedral angles at optimized geometries are 165±10°, 90±10° and 60±10° for Si and Ge. In addition to these minima Sn and Pb have an additional minimum at ~180°, and Pb has a minimum at 100±10°. Figure 17 shows the dependence of resonance integrals on the backbone dihedral angle for Si,[5] Ge, Sn, and Pb.

Table 1. Parameters of the Ladder C Model.

	α / eV	β_p / eV	β_g / eV	C_1 / eV	C_2 / eV
Si[5]	-6.10	-3.50	-1.10	0.11	-0.70
Ge	-6.10	-3.09	-1.07	0.17	-0.69
Sn	-6.28	-2.39	-1.05	0.16	-0.55
Pb	-6.41	-1.68	-1.12	0.20	-0.59

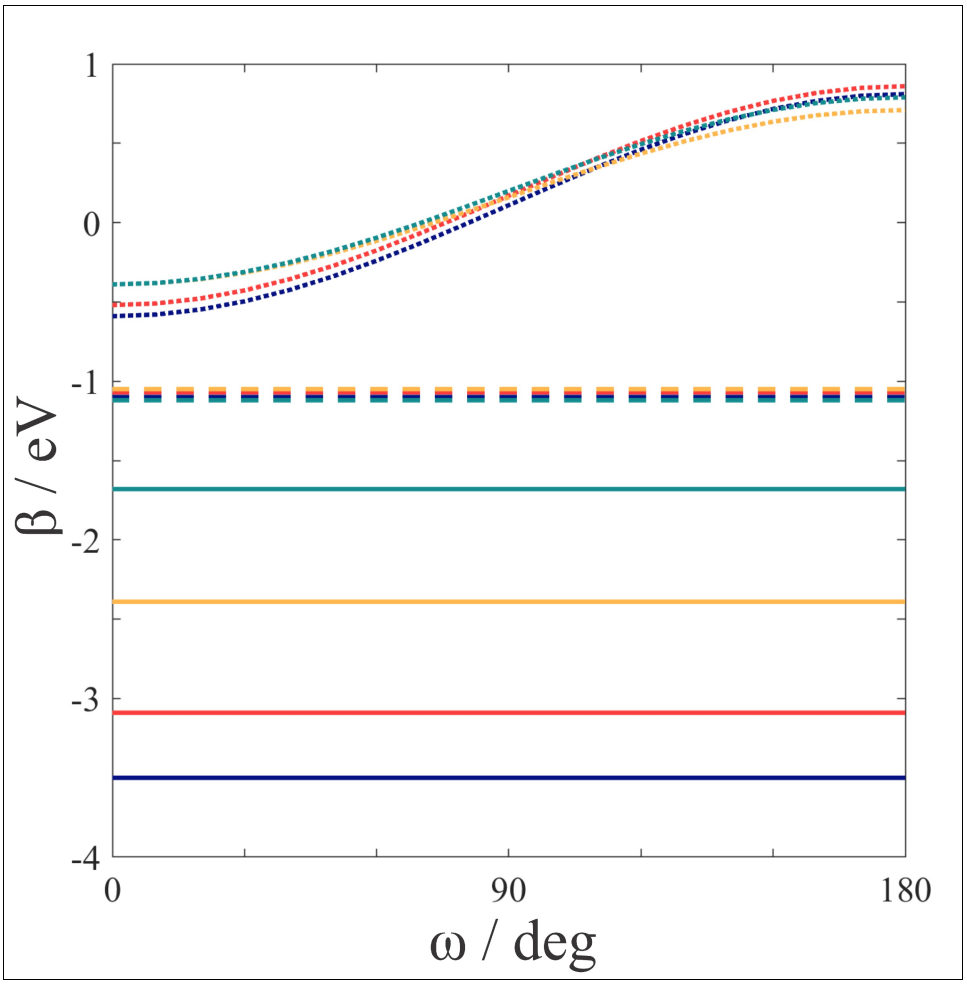


Figure 17. Conformational dependence of primary (full lines), geminal (dashed lines), and vicinal (dotted lines) resonance integrals in the Ladder C model for Si (dark blue),[5] Ge (red), Sn (yellow), and Pb (green).

Agreement between the MO energies and wave functions obtained from the Ladder C calculations and those obtained from HF calculations is very good (Table 2). The average RMS deviations in MO energies are on the order of 10^{-1} eV. The agreement of the orbitals can be judged by the overlap of the Ladder C MOs with the HF MOs expressed in the NHO basis, which is typically around 0.8 for the top 50% of occupied Ladder C orbitals. It appears that the Ladder C model provides a reasonable representation of the HF results at local equilibrium geometries for the skeletal bonding orbitals for all four choices of the element X. Figure 18 shows comparison between the Ladder C and HF orbital energies.

Table 2. Comparison of Ladder C and HF results.

	orbital energy RMS / eV	average overlap between LC and HF orbitals
Ge	6×10^{-2}	0.84
Sn	5×10^{-2}	0.81
Pb	8×10^{-2}	0.79

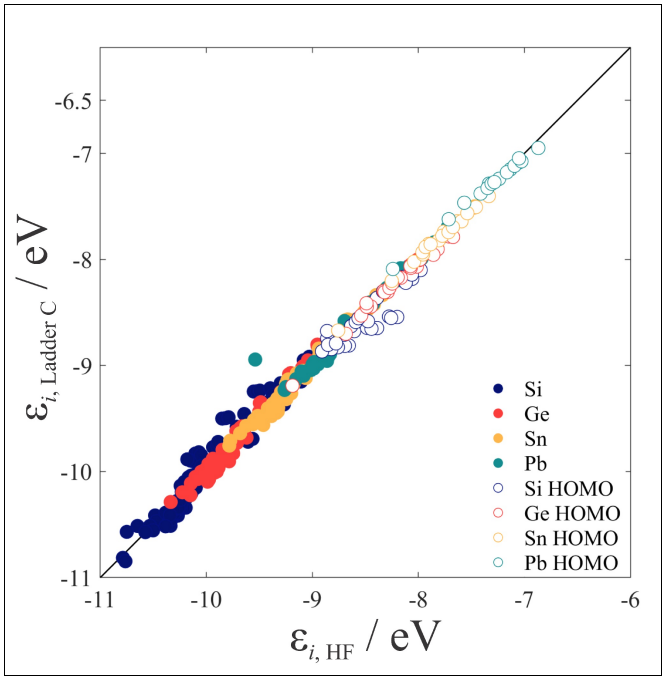


Figure 18. Comparison between energies of occupied HF and corresponding Ladder C orbitals for Si_nMe_{2n+2} (dark blue), Ge_nMe_{2n+2} (red), Sn_nMe_{2n+2} (yellow), and Pb_nMe_{2n+2} (green). Empty circles correspond to the energy of the HOMO, while full circles represent other occupied orbitals.

3.3.2. DFT calculations on infinite helices

Geometry optimizations were constrained by the choice of a line group, which affected molecular parameters. Bond lengths are found to be slightly longer than in molecules, with typical values of XX bond being 2.37 Å for Si, 2.41 Å for Ge, 2.82 Å for Sn, and 2.93 Å for Pb. In conformers with dihedral angles larger than $\sim 40^\circ$ bond angles are similar to the ones found in finite molecules: around $113 \pm 5^\circ$ for Si and Ge, and $112 \pm 5^\circ$ for Sn and Pb. When dihedral angles are small, the constrains of line group combined with the steric interactions between lateral methyl groups lead to an increase in valence angles. In this conformers, valence angles can reach values up to 132°.

3.3.3. Ladder C model for an infinite regular helix

A regular helix is the helix in which the parameters connecting translational unit cells are equal to the parameters connecting roto-translational units within the unit cell. Analytical solutions for Ladder C model can be found in the infinite chain limit with cyclic boundary conditions for both roto-translational and translational unit cell. We choose to use smaller roto-translational unit cell because it allows us to treat helices belonging to different line groups, characterized by distinct values of N_1 and N_2, on equal footing, as conformers of the same compound.

We choose a (roto-translational) unit cell that contains two hybridized atomic orbitals, χ_A and $\chi_{B,}$ pointing at each other and involved in primary bonding (Figure 19). The topology of orbital interactions within the infinite system resembles that of a ladder and gave the model its name. It

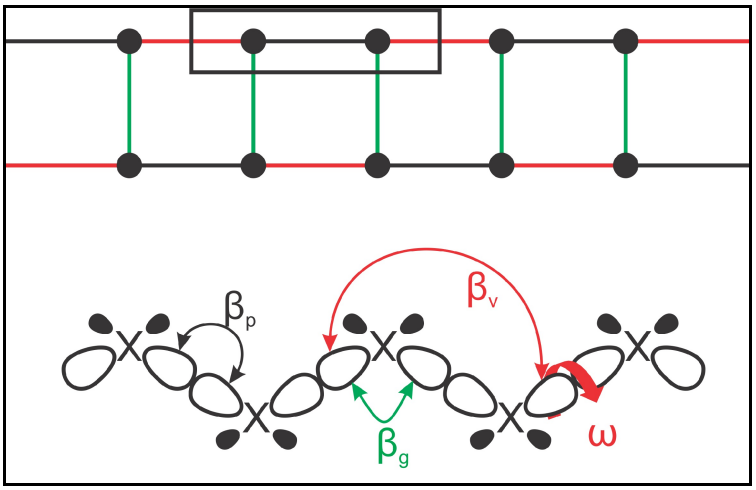


Figure 19. Top: The "ladder" representation of the Ladder C model - hybrid orbitals (full black circles) can interact via primary (black lines), geminal (green lines), and vicinal (red lines) interactions. The unit cell (boxed) contains two hybrids forming a chemical bond. Bottom: The chain representation of the Ladder C model: the interactions between hybrids (elliptical shapes) are shown via black (primary), green (geminal) and red (vicinal) arrows.

consists of two side pieces containing alternating primary (β_p) and vicinal (β_v) interactions and of rungs that allow the side pieces to communicate through geminal interactions (β_g). Each side-piece contains half of the primary XX bonds present in the molecular chain.

Molecular orbitals $\psi(k')$ are chosen as linear combinations of two Bloch waves, $\varphi_A(\boldsymbol{k}')$ and $\varphi_B(\boldsymbol{k}')$, located on the different sides of the ladder, each of which is a sum over all atomic orbitals χ_A and χ_B, respectively:

$$\psi(\boldsymbol{k}') = c_A\varphi_A(\boldsymbol{k}') + c_B\varphi_B(\boldsymbol{k}'), \tag{26}$$

$$\varphi_A(\boldsymbol{k}') = N^{-½}\sum_{m=0}^{N-1} e^{i\boldsymbol{k}'m}\,\chi_{Am}, \tag{27}$$

$$\varphi_B(\boldsymbol{k}') = N^{-½}\sum_{m=0}^{N-1} e^{i\boldsymbol{k}'m}\,\chi_{Bm}, \tag{27}$$

where N is the number of (roto-translational) unit cells in a chain, index m goes over all unit cells, $\boldsymbol{k}' = 2\pi n/Na$ is pseudo-wave vector, a is length of one-dimensional unit cell, and n is an integer. When pseudo-wave vector is used, the periodicity in the reciprocal space changes: the energy bands have a $2N_1\pi$ period. Values of $\boldsymbol{k}'$ between $-N_1\pi$ and $N_1\pi$ lie within a Jones zone.[46] The eigenvalues of the Ladder C Hamiltonian are determined by equation 28:

$$\varepsilon_{\pm}(\boldsymbol{k}') = \alpha \pm [\beta_p^{\,2} + \beta_{g2} + \beta_{v2} + 2\beta_p\,\beta_g\cos(\boldsymbol{k}') + 2\beta_v\,\beta_g\cos(\boldsymbol{k}') + 2\beta_p\,\beta_v\cos(2\boldsymbol{k}')]^{1/2}, \tag{28}$$

where $\varepsilon_-(\boldsymbol{k}')$ and $\varepsilon_+(\boldsymbol{k}')$ are the energies of the valence and conduction band, respectively, α is the Coulomb integral, and ω ranges from 0° to 180°. As explained above, we expect the Ladder C model to be valid only for the bonding orbitals and we shall not deal with the conduction band. With α as the energy zero and β_p as the energy unit, the energy and the eigenvectors for the valence band become:

$$\varepsilon_{gv}(\boldsymbol{k}') = -[1 + g^2 + v^2 + 2g\cos(\boldsymbol{k}') + 2gv\cos(\boldsymbol{k}') + 2v\cos(2\boldsymbol{k}')]^{1/2}, \quad (29)$$

$$\psi(\pm\boldsymbol{k}') = [(1+ge^{-i\boldsymbol{k}'} + ve^{-2i\boldsymbol{k}'})^{1/2}\varphi_A(\boldsymbol{k}') \pm (1+ge^{i\boldsymbol{k}'} + ve^{2i\boldsymbol{k}'})^{1/2}\varphi_B(k')]/[2(1+ge^{-i\boldsymbol{k}'} + ve^{-2i\boldsymbol{k}'})]^{1/2}, \quad (30)$$

where $g = \beta_g/\beta_p$ and $v = \beta_v/\beta_p$ define a two-dimensional parameter space $[g,v]$, in which g and v are a function of the choice of the backbone element and v depends on the dihedral angle ω. Since $\beta_p < 0$, the value of g is always positive, whereas the value of v is positive for tight helices, goes through zero near a helix dihedral angle of 90°, and is negative for loose helices. There are two main mechanisms of electron delocalization in σ-bondend molecules, σ-conjugation, the delocalization through geminal intercations, and σ-hyperconjugation, the delocalization through vicinal interactions. The extent of delocalization in a molecule is determined by interactions between the two mechanisms, which depends on the sign of v, and relative strengths of σ-conjugation, measured by g, and σ-hyperconjugation, measured by v.

As shown in Figure 20, the orbitals $\psi(\pm\boldsymbol{k}')$ have the simplest form at three points in the Jones zone, where the absolute value of all the coefficients on atomic orbitals is equal to $1/(2N)^{-1/2}$: (i) $\boldsymbol{k}' = 0$ (Γ point): the orbital ψ(Γ) has no nodes; (ii) $\boldsymbol{k}' = \pm N_1\pi/2$ (X" point): in the degenerate pair of orbitals, ψ(X") and ψ(−X"), there are no nodes across primary interactions, but there is a node across every other geminal and every vicinal interaction; (iii) $\boldsymbol{k}' = \pm N_1\pi$ (X' point): in the orbital ψ(X') = ψ(−X'), there is a node across all geminal interactions and no nodes across primary and vicinal interactions. The simplified form of the orbitals at $\boldsymbol{k}' = \pm N_1\pi/4$ (±X''' point) and $\pm 3N_1\pi/4$ (±X''''

point), in which vicinal interactions cancel out perfectly, is also shown in Figure 20. At other position in the $\boldsymbol{k'}$ space, the orbitals $\psi(\pm\boldsymbol{k'})$ have a more complicated form, in which the absolute value of orbital amplitude varies along the chain.

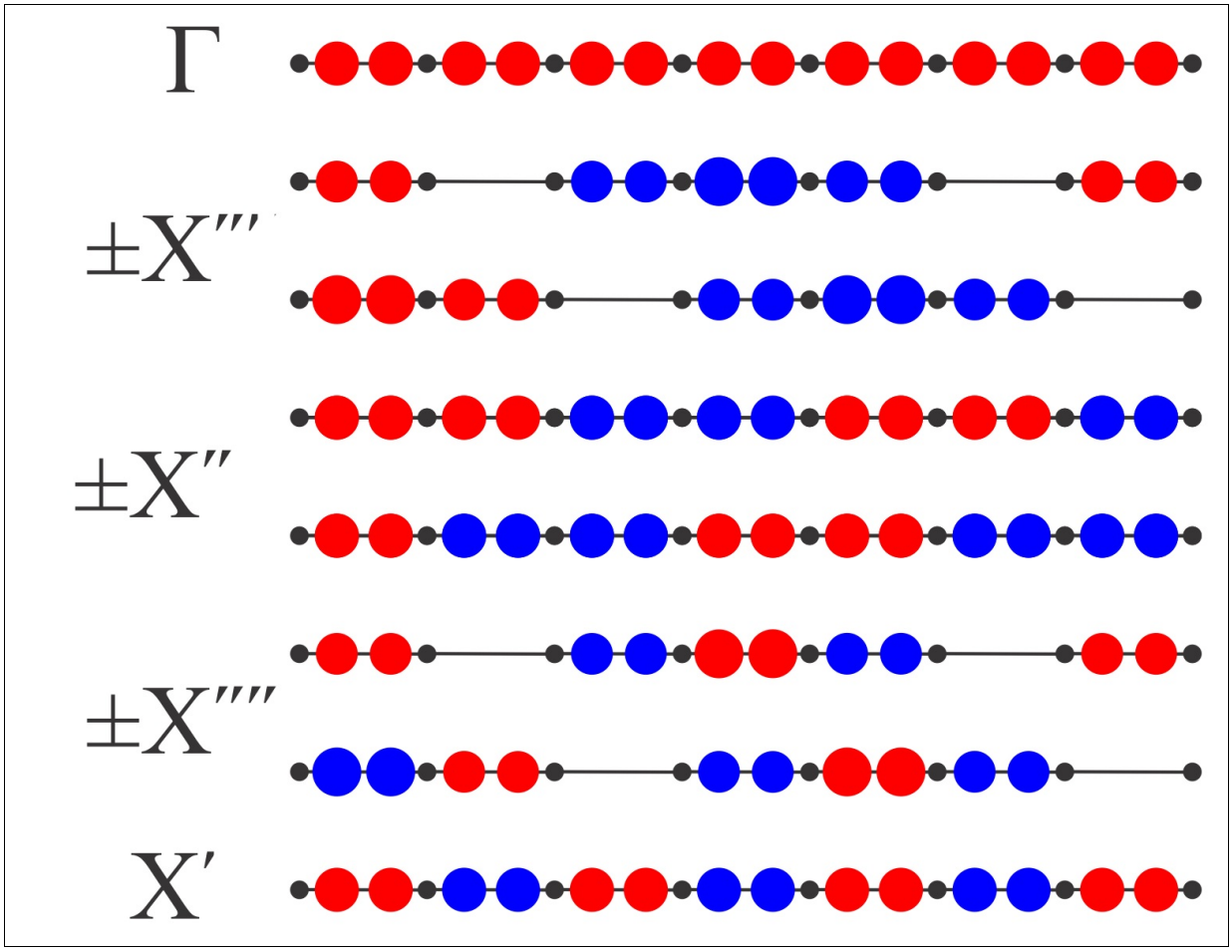


Figure 20. Schematic representation of crystal orbitals (CO) at the Γ, ±X‴, ±X″, ±X⁗, and ±X′ points. Atomic centers are represented via black circles, bonds via full lines, and the amplitude (size) and the sign (red for positive and blue for negative) of the CO coefficients on hybrids are represent via full non-black circles.

3.3.4. Comparison between Ladder C and DFT results

The left side of Figure 21 shows calculated valence bands of $(SiMe_2)_\infty$, $(GeMe_2)_\infty$, $(SnMe_2)_\infty$, and $(PbMe_2)_\infty$ conformers plotted within the Jones zone. The right side of Figure 21 shows corresponding Ladder C results. The DFT bands, calculated within the FBZ, are unfolded to give Jones zone band structure: N_1 bands in the FBZ give a smooth Jones-zone band. X' point is located at $\boldsymbol{k'} = N_1\pi$, where N_1 is a number of roto-translational unit cells in the translationally invariant unit cell and has a different value of for different conformers. X" point is located at $\boldsymbol{k'} = N_1\pi/2$ and corresponds to the center of the Jones zone.

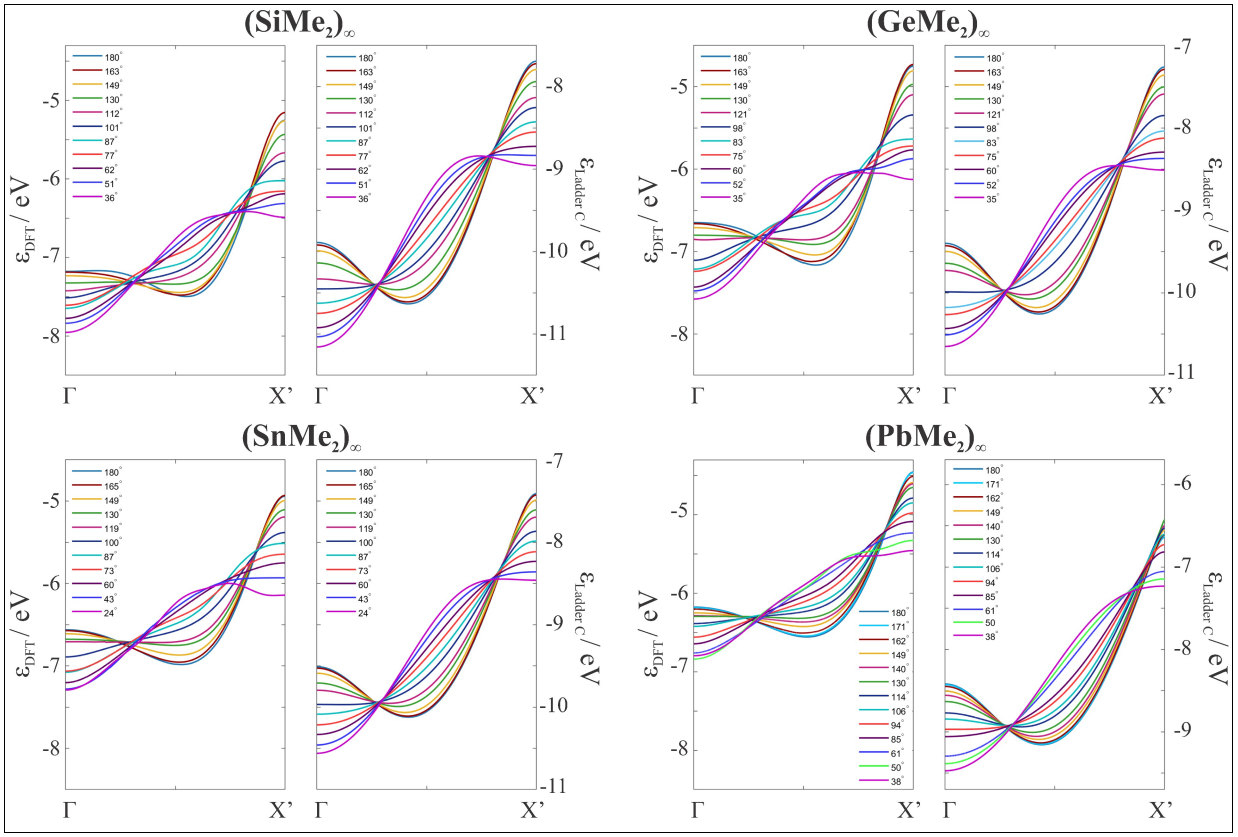


Figure 21. Valence bands structures of conformers of $(SiMe_2)_\infty$, $(GeMe_2)_\infty$, $(SnMe_2)_\infty$, and $(PbMe_2)_\infty$ calculated with DFT (on the left) and Ladder C (on the right) models, plotted in the Jones zone.

The valence band structures show good qualitative agreement between the Ladder C and DFT models. Regardless of method and backbone element X, the band structures in Figure 21 show similar traits. At large backbone dihedral angles ω the valence bands have a global maximum at the X' point, a local maximum at the Γ point, and a global minimum close to the X" point. As ω decreases, the global minimum shifts farther from the X" point towards the Γ point, leading to a valence band that has a maximum at the X' point and a minimum at the Γ point. As ω decreases even more, the band maximum shifts from the X' point towards the X" point. The valence bands of conformers with small dihedral angles are characterized by a local minimum at the X' point, a global minimum at the Γ point, and a maximum located between the X" and X' points. Smooth change of the valence band shape with decrease in the backbone dihedral angle is accompanied by flattening of the band in the region of the change (e.g. when a minimum shifts from the X" to Γ point, the band flattens between these points). The differences between models, such as the larger width of Ladder C bands and additional broad plateau in DFT bands, are caused by interactions of sigma backbone band with lower energy bands that are absent in the Ladder C model. As Ladder C model was parameterized to give good description of the frontier orbitals, there is a greater error in calculation of the energy of lower-lying orbitals, which is partially reflected in larger width of Ladder C bands. Additionally, the interactions with the lower energy bands push the bottom of the valence band to higher energies, which reduces the width of DFT bands. The largest differences occur at dihedral angle range from ~50 to ~120°. Mixing of backbone bonding orbitals of locally σ and locally π character is the strongest in this region, where the absence of a molecular symmetry plane is most evident. Moreover, in this range of angles delocalization is suppressed by the near absence of vicinal interactions, shifting the valence band to lower energies, where these additional interactions are more

likely. However, they do not affect orbitals close to the Fermi level, which determine physical and chemical behavior of solids.'

3.3.5 Measures of electron delocalization

To compare infinite helices with molecules, we need a measure of electron delocalization in extended systems. Effective mass of an electron in the conduction band or a hole in the valence band gives a prediction of the ease with which the electron (hole) can move through a crystal. Keeping in mind that electron delocalization in molecules leads to electrons (holes) that are not located in a single bond or on a single atom but are free to be in the other parts of the molecule, we adopt the effective mass as a good measure of electron delocalization in a crystals. We calculate the effective mass from the band structure, acknowledging that additional interactions within a crystal, such as phonon scattering, can farther decrease the mobility. As the top of the Jones zone valence band is composed of hybrid orbitals in XX σ bonds, we choose the effective hole mass as a good measure of the extent of σ-electron delocalization.

In an infinite chain, the effective hole mass m_h is defined as:

$$m_h = - \hbar^2 / [a^2 \partial \varepsilon_{gv}(\boldsymbol{k})^2 / \partial^2 \boldsymbol{k}|_{\boldsymbol{k} = \boldsymbol{k}max}] \tag{31}$$

where a is the unit cell length and $\partial \varepsilon_{gv}(\boldsymbol{k})^2 / \partial^2 \boldsymbol{k}|_{\boldsymbol{k} = \boldsymbol{k}max}$ is the second derivative of the energy with respect to the wave vector, evaluated at the band maximum. When we use roto-translational symmetry, a is the distance between roto-translational unit cells, and the derivative is taken with the respect to the pseudo-wave vector, $\boldsymbol{k'}$. The effective hole mass becomes:

$$m_h = - \hbar^2 / [a^2 \partial \varepsilon_{gv}(\boldsymbol{k'})^2 / \partial^2 \boldsymbol{k'}|_{\boldsymbol{k'} = \boldsymbol{k'}max}]. \tag{32}$$

In the Ladder C model, stationary points are found when the first derivative with respect to the pseudo-wave vector:

$$\partial\varepsilon_{gv}(\boldsymbol{k}')/\partial\boldsymbol{k}' = -[ga\sin(\boldsymbol{k}') + gva\sin(\boldsymbol{k}') + 2va\sin(2\boldsymbol{k}')][1 + g^2 + v^2 + 2g\cos(\boldsymbol{k}') + 2gv\cos(\boldsymbol{k}') + 2v\cos(2\boldsymbol{k}'))]^{-1/2} \quad (33)$$

is zero and occur at $\boldsymbol{k}' = 0$, $\boldsymbol{k}' = \cos^{-1}[-g(1 + v)/4v]$, and unless $g = 1 + v$, also at $\boldsymbol{k}' = \pm\pi$. Evaluation of the second derivative:

$$\partial\varepsilon_{gv}(\boldsymbol{k}')^2/\partial^2\boldsymbol{k}' = -\{a^2[1 + g^2 + v^2 + 2g(1 + v)\cos(\boldsymbol{k}') + 2v\cos(2\boldsymbol{k}')][g(1 + v)\cos(\boldsymbol{k}') + 4v\cos(2\boldsymbol{k}')] + a^2[g + gv + 4v\cos(\boldsymbol{k}')]^2\sin^2(\boldsymbol{k}')\}/\{[1 + g^2 + v^2 + 2g\cos(\boldsymbol{k}') + 2gv\cos(\boldsymbol{k}') + 2v\cos(2\boldsymbol{k}')]\}^{3/2} \quad (34)$$

shows that the stationary point at $\boldsymbol{k}' = 0$ is a maximum if $v < -g/(g+4)$ and a minimum for all other values of v when $g > 0$. The stationary point at $\boldsymbol{k}' = \cos^{-1}[-g(1 + v)/4v]$ is a maximum $v > g/|g-4|$ and a minimum for $v < -g/(g+4)$, if g is positive. The stationary point at $\boldsymbol{k}' = \pm\pi$ is a maximum at all $v \le g/|g-4|$ and a minimum when $v > g/|g-4|$, for $g > 0$.

Figure 22 shows effective hole mass calculated from DFT (full lines) and Ladder C (dashed lines) data for all choices of X as a function of the backbone dihedral angle ω. The agreement between Ladder C and DFT models is good. The smallest effective mass is predicted for large values of ω, and it increases as ω decreases. The effective mass reaches its largest values for intermediate values of ω, when the valence band maximum shifts from the X' point towards X" point and the top of band flattens. The value of ω at which this happens is not exactly the same in Ladder C and DFT models, which is a consequence of sensitivity of effective hole mass to the chosen values of g and v and is not of fundamental importance. σ-Electron delocalization is the strongest when the effective hole mass is at its minimum, for large values of the backbone dihedral angle, and electrons move easily through a helix. When the effective mass reaches infinity electrons are completely localized in individual σ-bonds.

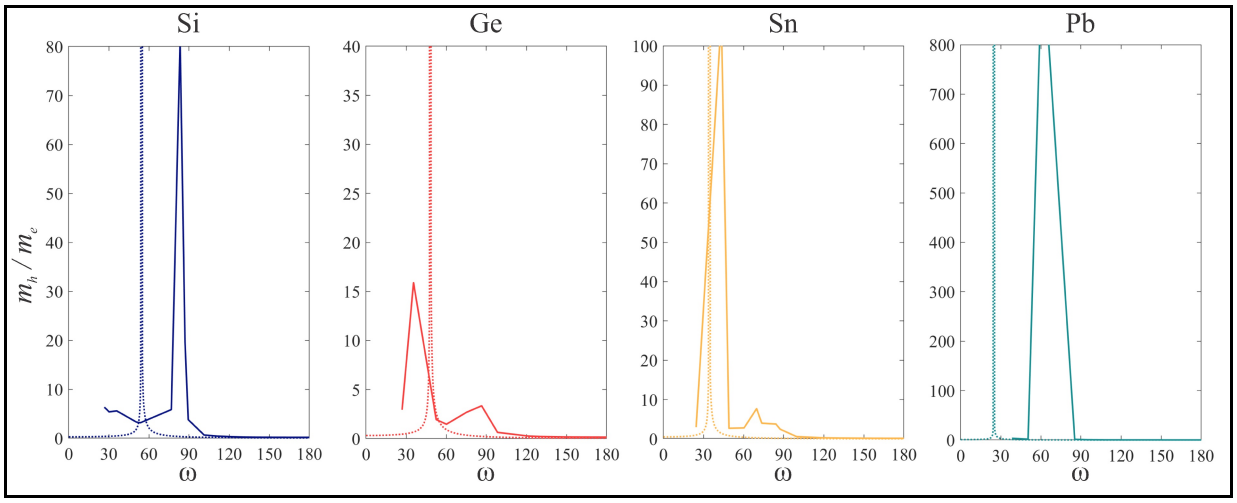


Figure 22. Effective hole mass in $(SiMe_2)_\infty$ (dark blue), $(GeMe_2)_\infty$ (red), $(SnMe_2)_\infty$ (yellow), and $(PbMe_2)_\infty$ (green) calculated with DFT (full lines) and Ladder C (dashed lines) models.

3.3.6. Understanding the origin of the results

To understand the origin of the results shown in Figures 21 and 22, we proceed along the lines adopted for oligosilanes,[73] and turn to perturbation theory. We separate Ladder C Hamiltonian into zeroth order Hamiltonian, which does not include geminal interactions (g = 0), and the perturbation that is the introduction of geminal interactions. This choice splits Ladder C chain into two non-interacting linear sub-chains of hybrids interacting alternately through primary and vicinal interactions, analogous to strongly alternating polyene. Each sub-chain contains half of XX bonds. Introduction of geminal interactions allows two sub-chains to interact, and recovers the effects of σ-conjugation.

When g = 0, the expressions 29, 33, and 34 become

$$\varepsilon_{g=0,v}(\boldsymbol{k}') = -[1 + v^2 + 2v\cos(2\,\boldsymbol{k}')]^{1/2}, \tag{35}$$

$$\partial\varepsilon_{g=0,v}(\boldsymbol{k}')/\partial\boldsymbol{k}' = [2v\sin(2\boldsymbol{k}')]/[1 + v^2 + 2v\cos(2\boldsymbol{k}')]^{1/2}, \tag{36}$$

$$\partial\varepsilon_{g=0,v}(\boldsymbol{k}')^2/\partial^2\boldsymbol{k}' = \{2v[2(v^2 + 1)\cos(2\boldsymbol{k}') + v(3 + \cos(4\boldsymbol{k}')]\}/[1 + v^2 + 2v\cos(2\boldsymbol{k}')]^{3/2}. \tag{37}$$

The first derivative has three stationary points at the Γ, X", and X' points (Figure 23A):

$$\varepsilon_{g=0,v}(\Gamma) = \varepsilon_{g=0,v}(X') = -|1 + v|, \tag{38}$$

$$\varepsilon_{g=0,v}(X'') = -|v - 1|. \tag{38}$$

Figure 23A shows resulting band structures for prototypical values of v = 0.2, 0, and -0.2. When $v < 0$, the stationary points Γ and X' correspond to maxima, and a minimum is located at X". The opposite is true when $v > 0$. In the special case of $v = 0$, the stationary point at X" disappears, and degeneracy between the X' and Γ points is broken: there is a maximum at the X' point, and a minimum at the Γ point. The trends can be understood in terms of nodal structure of the valence band eigenvectors at stationary points. The eigenvectors in the valence band have no nodes across primary interactions, and relative energy of the orbitals is dictated by sign of v: ψ(Γ) and ψ(X') have no nodes across vicinal interactions (Figures 20 and 23) and they are the most stable orbitals when $v > 0$ and the least stable orbitals when $v < 0$; the opposite is true for ψ(X"), which has a node

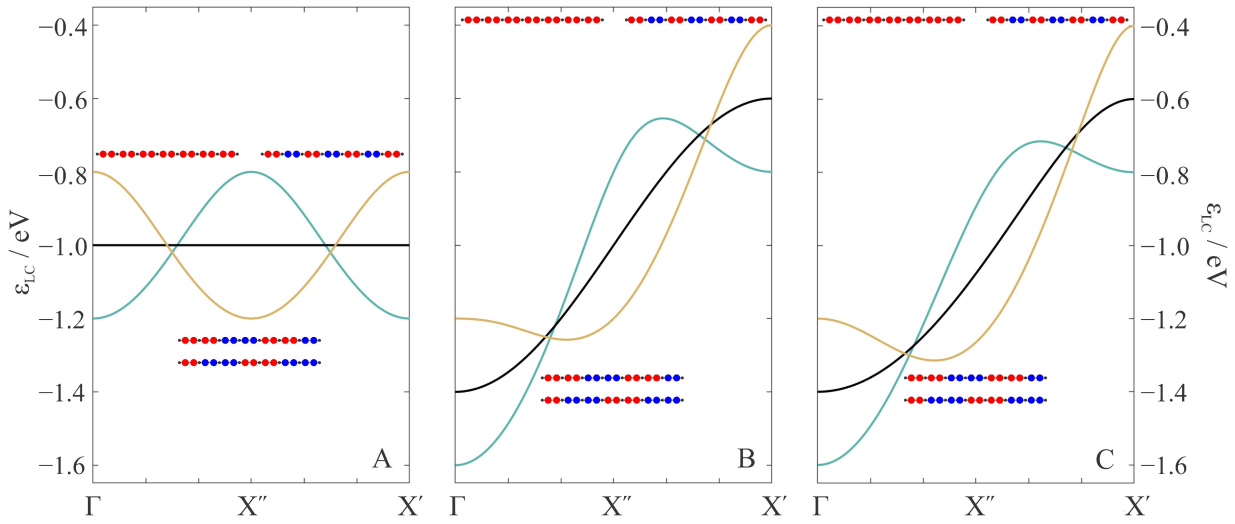


Figure 23. Zeroth order (A), first order perturbation theory (B), and exact Ladder C (C) valence band dispersion for $v = 0.2$ (green), $v = 0$ (black), $v = -0.2$ (gold), and $g = 0.4$ (B and C). Structure of ψ(Γ) and ψ(X') is shown schematically on the top of the band dispersion, while ψ(±X") is shown at the bottom.

through each vicinal interaction. The number of nodes across vicinal interactions is dictated by symmetry, and it increases from the Γ and X' points toward the X" point. The symmetry around the X" point is present because the zeroth-order Hamiltonian does not differentiate between in-phase (left of the X" point) and out-of-phase (right of the X" point) combination of orbitals on two sub-chains. Finally, when $v = 0$, the sub-chains become a set of perfectly localized, equivalent σ-bonds.

In the next step, we introduce geminal interactions, $g > 0$, perturbatively. The first order energy correction is given by:

$$\varepsilon'_{g\neq 0,v}(\boldsymbol{k'}) = -[g(1+v)\cos(\boldsymbol{k'})][1+v^2+2v\cos(2\boldsymbol{k'})]^{-1/2}. \quad (39)$$

The effects of the perturbation on the band structure are profound (Figure 23B), and we see a rise of three characteristic band structures seen in Figure 21. The symmetry around the X" point is broken as geminal interactions stabilize in-phase and destabilize out-of-phase combinations of the hybrids on two sub-chains. The magnitude of the orbital energy change increases with distance from X". Introduction of $g \neq 0$ will have the greatest effect on the energy of ψ(Γ) and ψ(X'), while, up to the first order approximation, ψ(X") will not change its energy at all. When $v < 0$, the resulting band has a global maximum at the X' point, additionally destabilized by introduction of geminal interactions, a stabilized local maximum at the Γ point, and a minimum that is shifted from the X" point to a smaller $\boldsymbol{k'}$ value. The flat band at $v = 0$ increases in width, as electrons are allowed to delocalize through geminal interactions. It has a maximum at the ψ(X') and a minimum at ψ(Γ), resembling the band dispersion of a linear polyene. Finally, when $v > 0$, the band structure will be characterized by stabilized minimum at the Γ point, destabilized minimum at X' point, and a maximum that is shifted from the X" point to a larger $\boldsymbol{k'}$ value.

The physical reason for this change can be found in the form of the eigenvectors: ψ(Γ) has no nodes across geminal interactions, and it is the most stabilized of all orbitals; ψ(X") has a node

across every other geminal interaction, leading to a perfect cancellation of stabilizing and destabilizing interactions, leaving orbital energy unchanged; ψ(X') has a node across every geminal interaction, and it will be the most destabilized of all orbitals. Number of nodes across geminal interaction increases from the Γ to X' point in symmetrical fashion. As other orbitals, initially close in energy to ψ(X"), change their energy the band maximum (when $v > 0$) or minimum (when $v < 0$) will shift from X" to some other $\boldsymbol{k'}$ value. The changes around the X" point are the most important for the hole delocalization when $v > 0$: as the perturbation gradually increases the energy of the orbitals that are on the right of ψ(X") the band maximum shifts towards the X' point, and the band flattens. When higher order terms are introduced, the orbital at ψ(X") changes its energy, but this change is small compared to the change in energy experienced by other orbitals. The simple explanation given by perturbation theory holds even for the full solutions, shown in Figure 21C.

The valence bands of different conformers will have a quasi-crossing points close to $\boldsymbol{k'} = \pm N_I\pi/4$ and $\pm 3N_I\pi/4$ (the X''' and X'''' points) . The origin of this phenomenon lies in the form of the wave-function at these points (Figure 20): there is equal number of stabilizing and destabilizing vicinal interactions along the chains, leading to the perfect cancellation of conformation-dependent interactions. As the orbital coefficients depend not only on the vicinal resonance integrals, but also on the primary and geminal ones, the quasi-crossing points at which the cancellation happens shift form the X''' and X'''' points to some other, nearby $\boldsymbol{k'}$ values. The exact position of the points depends on the parameters of the Ladder C model and on the DFT functional.

The effective hole mass can help us understand the influence of the perturbation on electron delocalization. At the zeroth order (Figure 24), m_h depends only on the amplitude of v, which dictates the strength of the interactions between neighboring sites, but not on the sign of v as the form of ψ(Γ) and ψ(X'), for $v < 0$, and ψ(X"), for $v > 0$, allow even delocalization along a sub-chain.

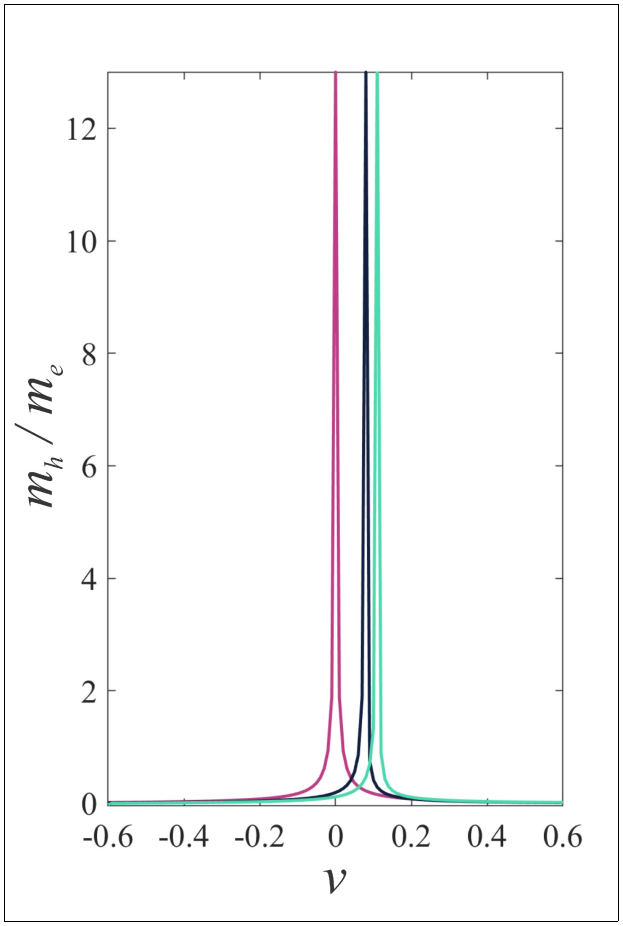


Figure 24. Effective hole mass as a function of v calculated from the Ladder C band structure at the zeroth order perturbation theory (pink), the first order perturbation theory (purple), and the exact solution (green), when $g = 0.4$.

The effective hole mass is infinite when $v = 0$, and the electrons in neighboring bonds do not interact. This occurs at dihedral angles ω = 80.96° for Si, ω = 76.59° for Ge, ω = 73.09° for Sn, and ω = 67.55° for Pb. When $g \neq 0$, the symmetry around $v = 0$ is removed. Introduction of geminal interactions leads to a new form of delocalization, the delocalization between sub-chains. The sign of v becomes relevant for an interplay between geminal and vicinal interactions: when there is constructive interference between the interactions, the delocalization is enhanced; the effective hole mass goes to infinity when the effects of geminal interactions perfectly cancel out the effects of vicinal interactions, and there is no delocalization in the chain.

3.3.7. Dependence of σ-electron delocalization on the backbone atom

In all compounds of the form $(XMe_2)_n$, X = Si, Ge, Sn, Pb, σ delocalization will depend on the conformation (Figure 21). There will be some differences: in silanes, the transition between σ delocalized and the σ localized behavior will happen already at ω close to 60°, while in plumbanes

the same transition will take place when ω is less than 25°. Silanes and germanes show strong dependence of σ delocalization on the chain conformation, while stannanes and plumbanes remain in σ delocalized regime even for ω= 30° and σ localization occurs only at small, probably physically not achievable values of ω.

Figure 25 shows three different regions, corresponding to three different types of band dispersion observed in Ladder C model for *g* between 0 and 1, and *v* between -0.6 and 0.6. The values of *g* and *v* in the light green region give the band dispersion where the maximum is at $\boldsymbol{k'} = \arccos(-g(1+v)/4v)$, the global minimum is at the Γ point, and the local one is at the X' point. The white region encloses *g* and *v* values for which the energy dispersion minimum is at the Γ point and the maximum is at the X' point. The *g* and *v* values in the gold region correspond to the energy dispersion which has the global maximum at the X' point, local one at the Γ point, and the minimum at $\boldsymbol{k'} = \arccos(-g(1+v)/4v)$. The dark blue line, $v = g-1$, shows the relationship between *g* and *v* necessary for the perfect delocalization effects, which leads to zero effective mass. The black line, $v = g/(g-4)$, gives all values of *g* and *v* that satisfy the condition for a perfect cancellation of the delocalization and infinite effective hole mass. Horizontal lines on the Figure 25 show the *g* and *v* values for $(XMe_2)_n$, X = Si, Ge, Sn, Pb.

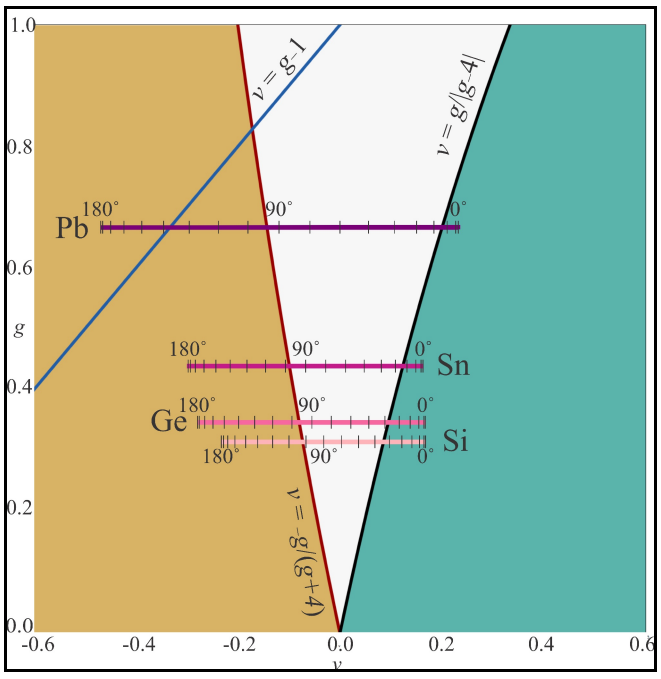


Figure 25. The [*g*,*v*] space.

σ-Electron delocalization is the strongest in conformers that have large dihedral angles and lie within gold region (loose helices). In loose helices, the delocalization is a result of cooperation between vicinal and geminal interactions, present when $v < -g/(g+4)$. The delocalization weakens in intermediate helices, which have dihedral angles within white region. The weakening is due to the opposing effects of geminal and vicinal interactions in this region. The cancellation between vicinal and geminal interactions is exact at $v = g/(g-4)$. After perfect cancellation, the effects of vicinal interactions win over geminal interactions, and a small amount of delocalization is present in the conformers that have dihedral angles within green region, called tight helices. As the strength of σ-bonds decreases from Si to Pb the relative strength of delocalization increases, which can be seen from elongation of the lines belonging to heavier elements in Figure 25.

Silicon. In silanes $g = 0.32$, and $v(\omega)$ ranges from -0.23, when $\omega = 180°$, to 0.17, when $\omega = 0$. When v is at its smallest value, both stronger σ-conjugation and weaker σ-hyperconjugation contribute to the electron delocalization, leading to efficient delocalization through the chain. The delocalized behavior smoothly converts to the localized behavior, as v increases in value, and the effects of σ-hyperconjugation partially cancel out the delocalization through σ-conjugation. For values of v close to zero, corresponding to dihedral angles approximately from 90° to 50°, σ-conjugation is the dominant mechanism of delocalization, and we see a dispersion analogue to the one seen in linear polyenes - the band maximum is located at the X' point and the minimum is at the Γ point. This is weakly delocalized transition region. When ω is smaller than 50°, σ-hyperconjugation is the dominant mechanism of delocalization. The effects of σ-hyperconjugation and σ-conjugation weaken as the highest occupied eigenstate is not located at the edge of the Jones zone but shifted towards smaller values of the wave vector.

Germanium. For germanes $g = 0.34$, and the range of $v(\omega)$ is from -0.27, for $\omega = 180°$, to 0.17, when $\omega = 0$. The behavior of germanes is similar to the behavior of silanes: loose helices, with backbone angle between 180° and 120° show strong σ delocalization, while the tight helices, with backbone angles between 50° and 0° behave like σ weakly delocalized systems. The transition between two delocalized regions happens through localized region for dihedral angles approximately between 90° and 50°.

Tin. The value for *g*, 0.44, is higher for stannanes than for silanes and germanes, because Sn-Sn bonds are significantly weaker than Si-Si and Ge-Ge bonds, while the geminal interactions stay approximately the same. The range of $v(\omega)$ values is from -0.30, for $\omega = 180°$, to 0.16, for $\omega = 0°$, which is similar to silanes and germanes. The importance of σ-conjugation increases greatly in these molecules. The conformational dependence of σ delocalization will be weaker than in silanes and germanes because σ-conjugation is stronger than conformational-dependent σ-hyperconjugation. The loose helix behavior will dominate for backbone angles from 180°to 100°, and the tight helix behavior will show only in syn and cisoid conformations (ω close to 0°). The transition region, where σ-hyperconjugation is weak or absent, can be seen when backbone angles are smaller than 100° but greater than 30°.

Lead. In plumbanes $g = 0.67$, and $v(\omega)$ is between -0.48 and 0.22. The effects of delocalization are the strongest in plumbanes because Pb-Pb bonds are the weakest. Results indicate that, unlike in other group 14 hydrides, the delocalization in plumbanes is the strongest when $\omega \sim 120°$ when Ladder C predicts perfectly delocalized system. σ-Conjugation is the dominant mechanical of delocalization for all values of ω greater than 30° and the tight helix behavior will show only for extremely small dihedral angles. Conformers with dihedral angles between 180° and

90° will be strongly delocalized, and the ones with smaller dihedral angles will show localized behavior.

3.4. Conclusions

The present work provides answers to the questions we asked at the beginning of the study and it has led to three conclusions: (i) The conformational dependence of σ-electron delocalization is present in polymers as well as in molecules. The effective hole mass is a sensitive measure of σ delocalization in extended systems, but it cannot provide information about the dominant mechanism of the delocalization. On the other hand, the shape of the valence band and the position of the band maximum in the Jones zone are indicators of the delocalization mechanism: when the band maximum is at the X' point the delocalization is dominated by σ-conjugation, and when the maximum is shifted towards smaller $\boldsymbol{k'}$ values the delocalization is dominated by σ-hyperconjugation. The intuitive explanation of the conformational dependence we provided for molecules translates to extended systems. (ii) σ-Electron delocalization is present in all heavier analogs of alkanes, $(XMe)_2$, where X = Si, Ge, Sn, Pb. (iii) Ladder C model is in a good agreement with PBE0/POB-TZVP calculations, and it is capable of providing a good description of the ground state properties of $(XMe)_2$ compounds.

Chapter IV

Conclusions

4.1. Summary

The present work has been motivated by the desire to understand electron delocalization in σ-bonded molecules. An intuitive explanation of the conformational dependence of σ delocalization in terms of simple models is provided through calculations and theoretical modeling.

The first part of the study, presented in Chapter II, focuses on oligosilanes, which are used as model systems due to the well-documented influence of their conformation on σ delocalization. The comparison of TD-DFT and experimental results for a series of all-[*t*] and all-[*ca*] conformers of Si_nMe_{2n+2}, for $n = 4$, 6, 8, and 10, has proven that TD-DFT method correctly reporduces both the strong chain-length dependence of the first singlet excitation energy in all-[*t*] conformers and its near chain-length independence in all-[*ca*] conformers. Furthermore, the comparison shows that TD-DFT can be used to compute vertical excitation energies of oligosilanes. It is shown that oligosilanes exist as two different chromophores with distinct properties, σ-delocalized conformers with large dihedral angles and σ-localized conformers with small dihedral angles, and an explanation of this phenomenon is provided in terms of a simple model. The change in electron delocalization can be understood through correlation diagrams between two limiting chromophores, all-[*a*] ($\omega = 180°$) and all-[*s*] ($\omega = 0°$): in a hypothetical system, in which there is no σ-conjugation, the HOMO in both chromophores is perfectly σ-hyperconjugated; however, the introduction of σ-conjugation enhances delocalization in all-[*a*] conformers and inhibits the delocalization in all-[*s*] conformers, in which the nature of the frontier orbitals changes to give a HOMO that is segmented into islands with a large electron density separated by regions of small electron density.

The second part of the study, presented in Chapter III, focuses on the effects of electron delocalization in *n*-polysilane and its heavier analoges, with germanium, tin, or lead as a backbone element. It is demonstrated that the effective hole mass can be used as a qualitative measure of electron delocalization in different conformers of $(XMe_2)_\infty$, X = Si, Ge, Sn, Pb, in which common measures of electron delocalization fail due to the extended nature of the system. Conformational dependence of electron delocalization was detected in all compounds. Simple modeling was used to show that the complex interplay between σ-conjugation and σ-hyperconjugation leads to delocalization in conformers that have large dihedral angles and localization in conformers that have small dihedral angles. An additional delocalized region of conformation space in which σ-hyperconjugation is the dominant mechanism of delocalization is found. This region is not physically accessible for $(XMe_2)_\infty$, X = Si, Ge, Sn, Pb compounds due to steric interactions. The results suggest a definition of a [*g*,*v*]-delocalization space which can be used to predict the extent of (de)localization in different compounds as well as the dominant mechanism of electron delocalization.

The conformational dependence of electron delocalization in oligo- and polysilanes, germanes, and stannanes can be used as a switch between two limiting behaviors, as demonstrated in an increasing number of experimental studies. The simple understanding of σ-electron delocalization and localization given in this work could guide and facilitate design of useful chromophores and molecular wires based on saturated molecules. Moreover, the explanations and methods presented here are a stepping stone for studying the complex phenomenon of σ delocalization in all saturated compounds.

4.2. Future Directions

The explanation of conformational dependence of σ delocalization presented in this work arises from the Ladder C model. During the course of this work, it was show that the Ladder C model can reproduce the predictions of higher level theoretical models, such as HF and DFT, but the model itself still has significant limitations. For example, it cannot be applied to alkanes, the most abundant saturated molecules, because of similar electronegativity of the backbone atoms and lateral substituents. Furthermore, the model does not provide a good description of excited states in molecules and conduction band in solids, which also depend on the presence of lateral substituents. The restrictions of the Ladder C model are fixed in a more complex Ladder H model that includes 4 sp^3 hybrid orbitals on the backbone atoms and an orbital per lateral substituent. Due to its complexity, the Ladder H model was disregarded in the present attempts to gain simple understanding of σ-electron delocalization. However, several questions that arose during the course of this work require the use of the Ladder H model: (i) The Ladder C model cannot properly describe the response of a system to an increase of chain length in the regular oligosilanes in which dihedral angle alternates between 180° and 0°, while preliminary results show that the Ladder H model captures the trend correctly. (ii) DFT and Ladder H predict an existence of localized states in all-[*c*] oligosilanes. These states are not present in the Ladder C model, and any study of their nature would have to rely on the Ladder H model. (iii) Finally, the apparent lack of conformational dependence of electron delocalization in alkanes cannot be captured by the Ladder C model, because the delocalization in alkanes is strongly influenced by lateral substituents. Future work on σ-electron delocalization should be based on the Ladder H model, which can help answer the remaining questions.

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Appendix

for

Conformational Dependence of σElectron Delocalization in the Catenae X_nMe_{2n+2}, X = Si, Ge, Sn, and Pb

Thesis written by Milena Jovanović and directed by Professor Josef Michl

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Calculated band structures and densities of states

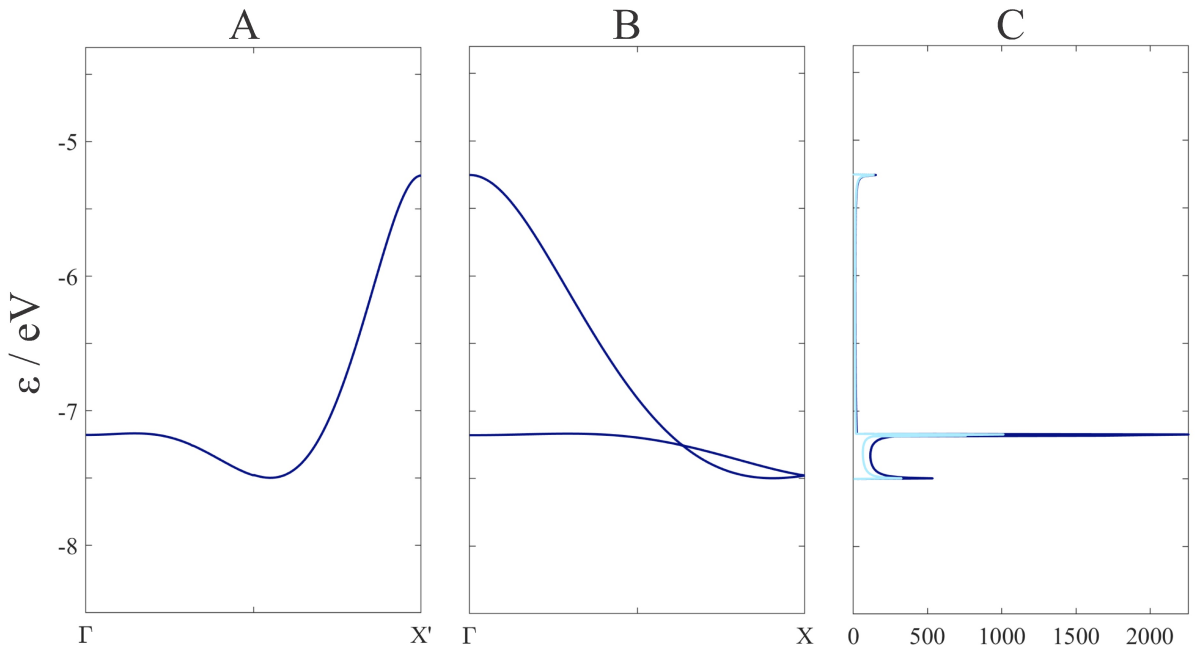

Figure A1. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[180.0]-$(SiMe_2)_\infty$

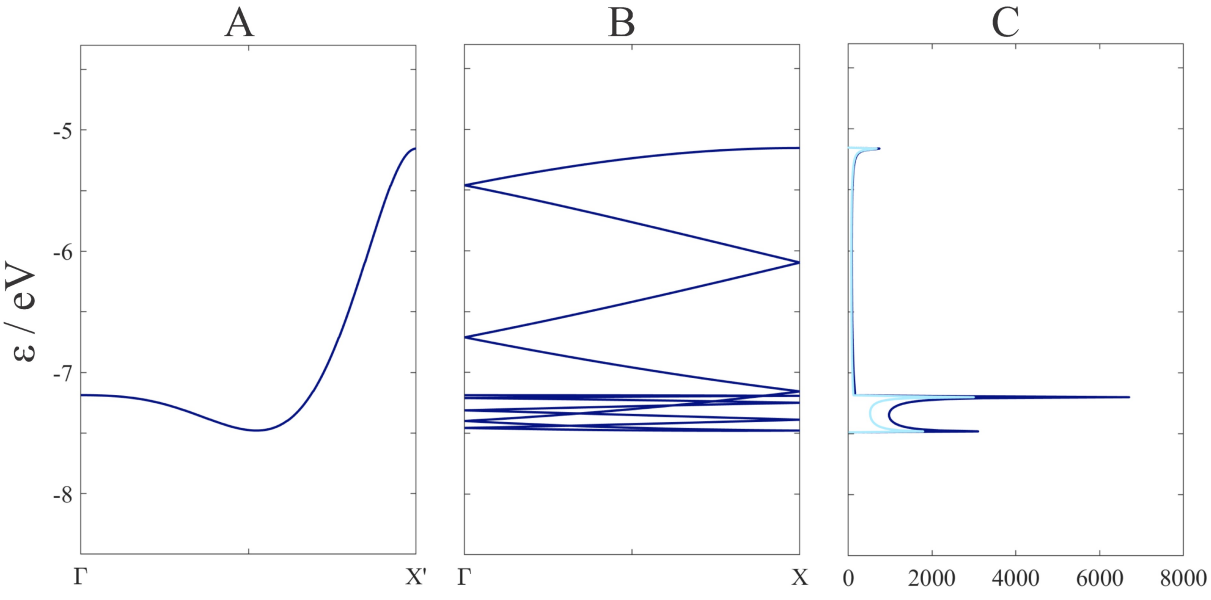

Figure A2. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[163.0]-$(SiMe_2)_\infty$

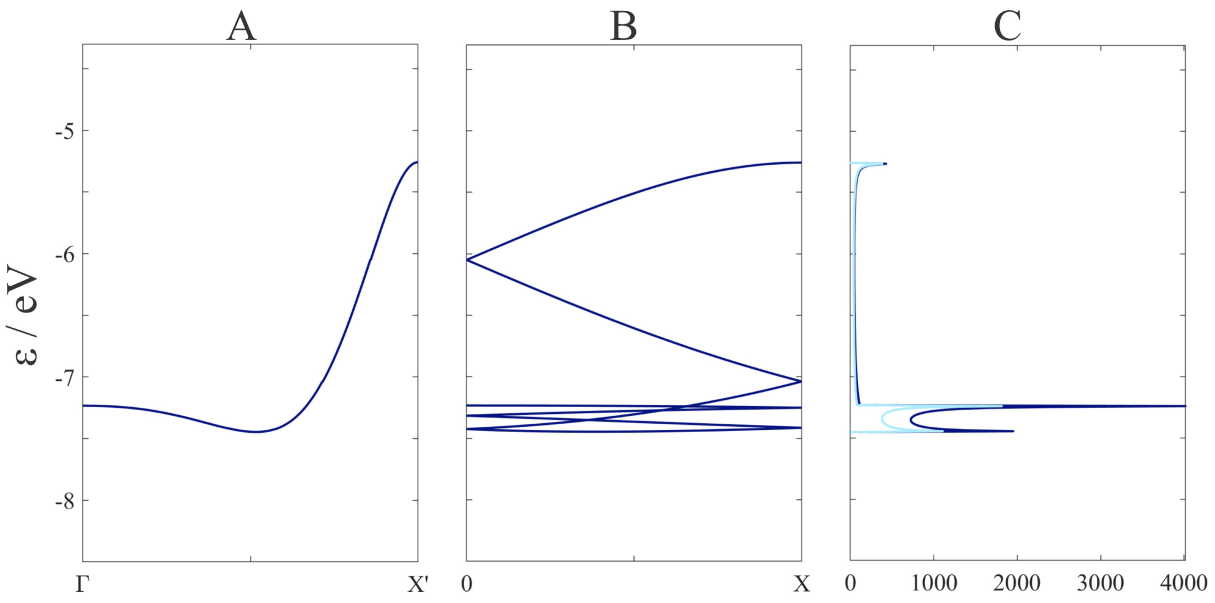

Figure A3. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected (light blue) Si density of states (C) for *all*-[148.0]-$(SiMe_2)_\infty$

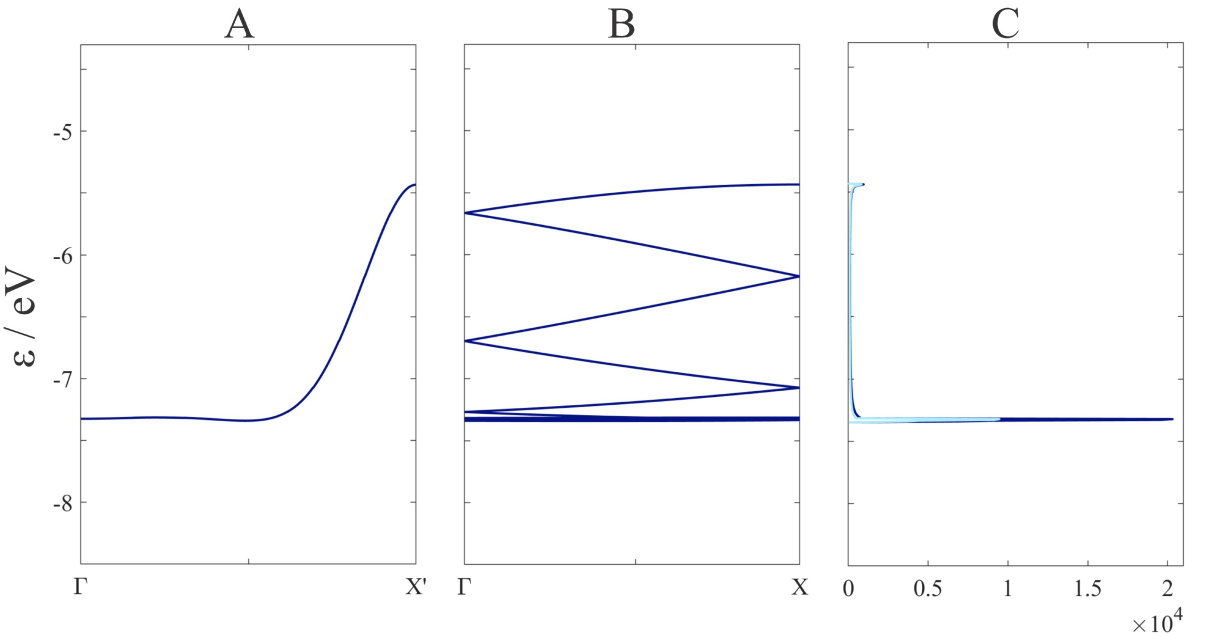

Figure A4. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[130.2]-$(SiMe_2)_\infty$

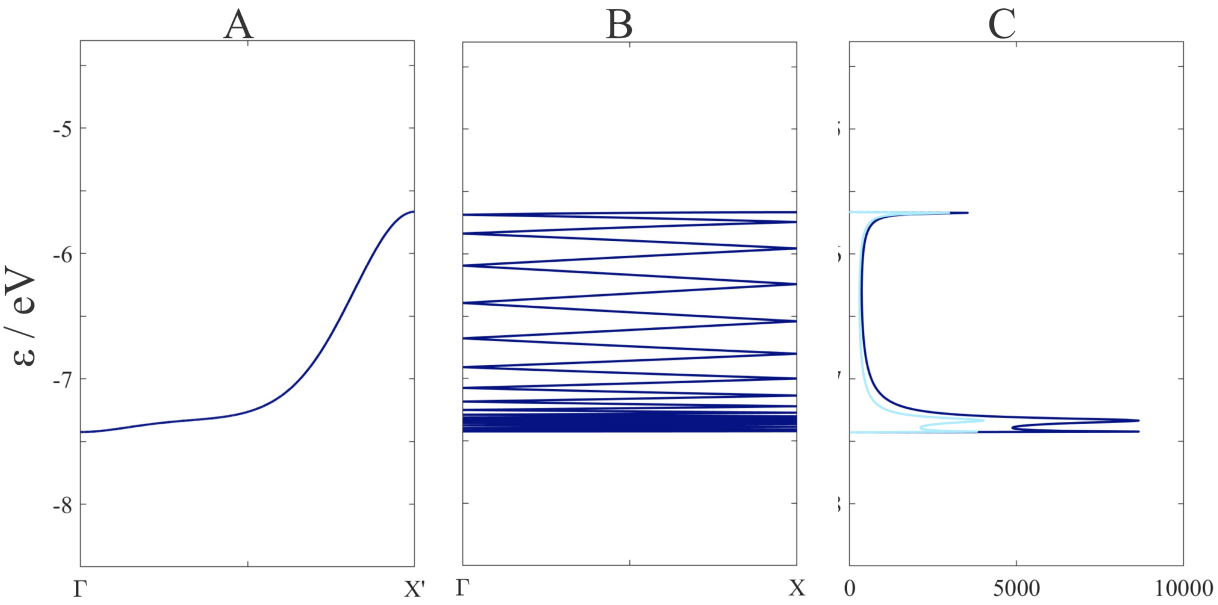

Figure A5. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[111.6]-$(SiMe_2)_\infty$

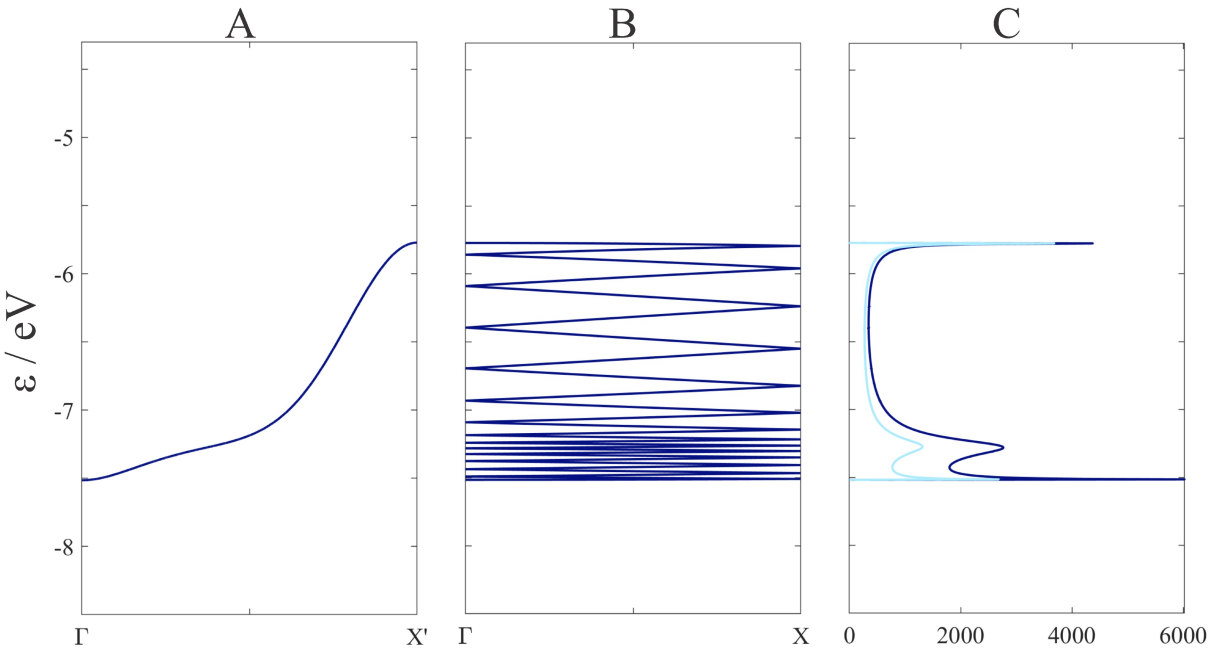

Figure A6. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[101.3]-$(SiMe_2)_\infty$

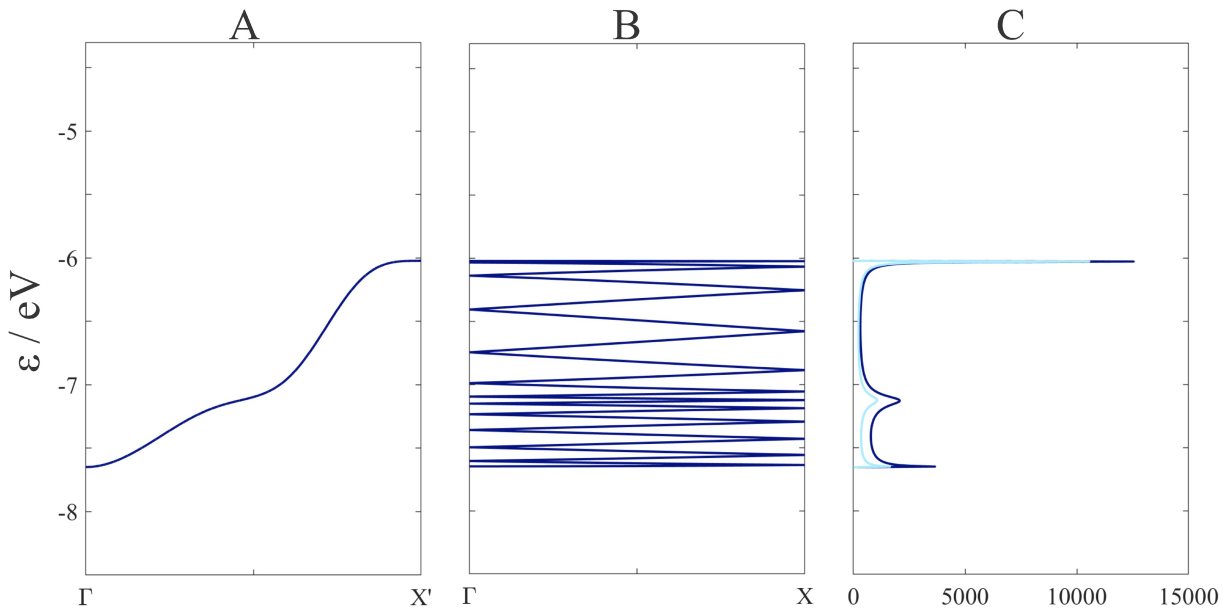

Figure A7. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[86.9]-$(SiMe_2)_\infty$

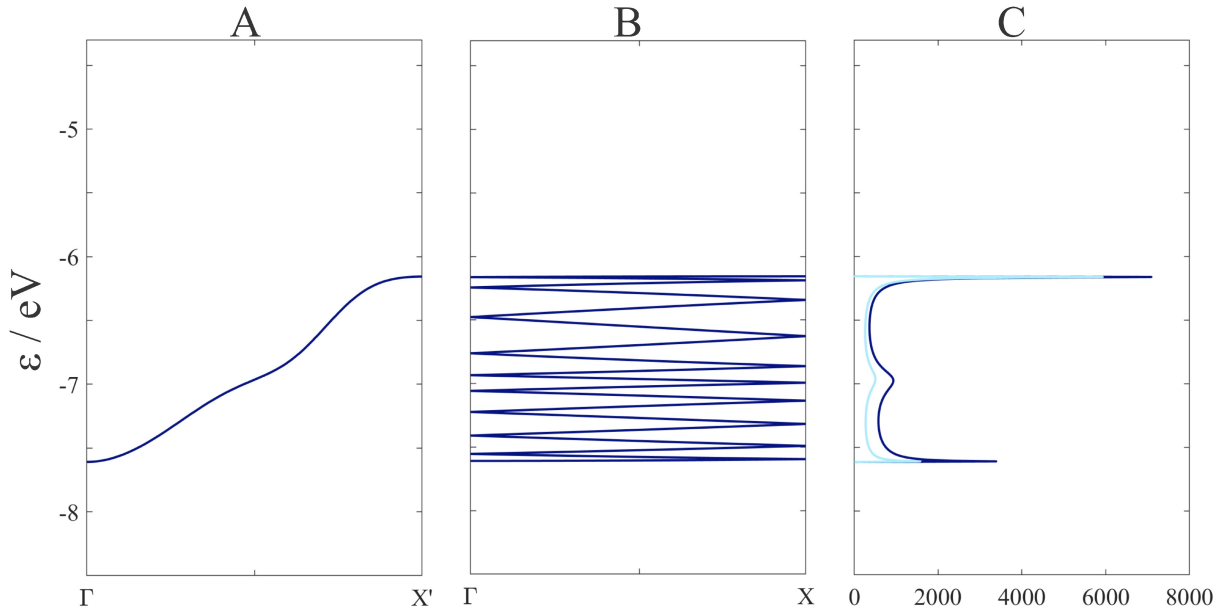

Figure A8. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[76.7]-$(SiMe_2)_\infty$

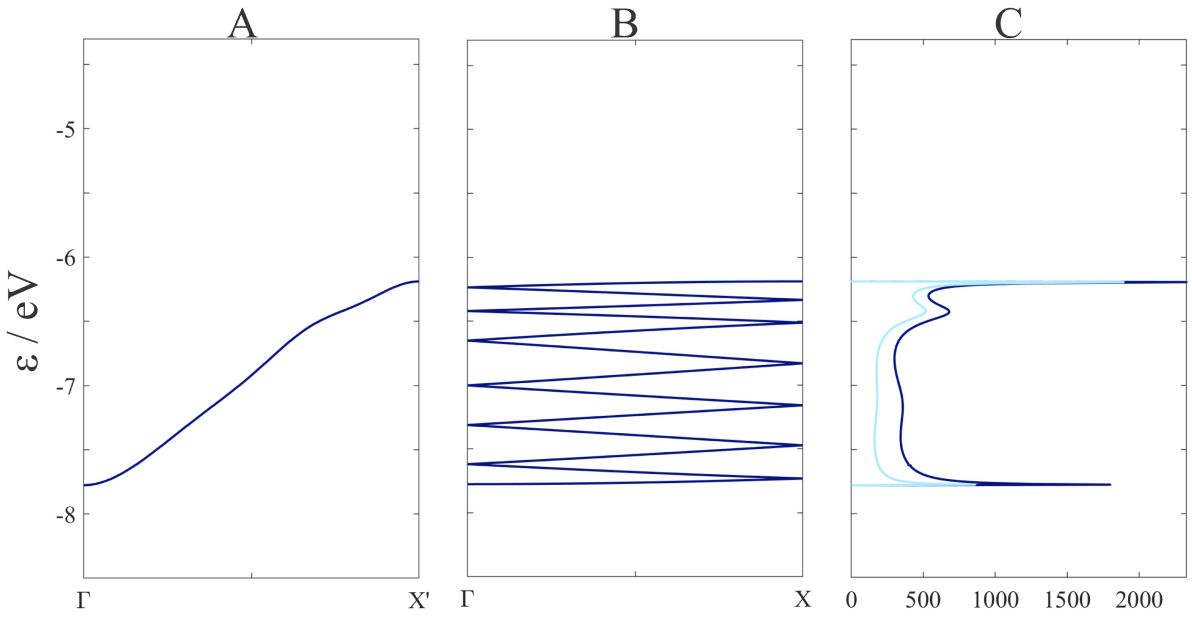

Figure A9. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[61.5]-$(SiMe_2)_\infty$

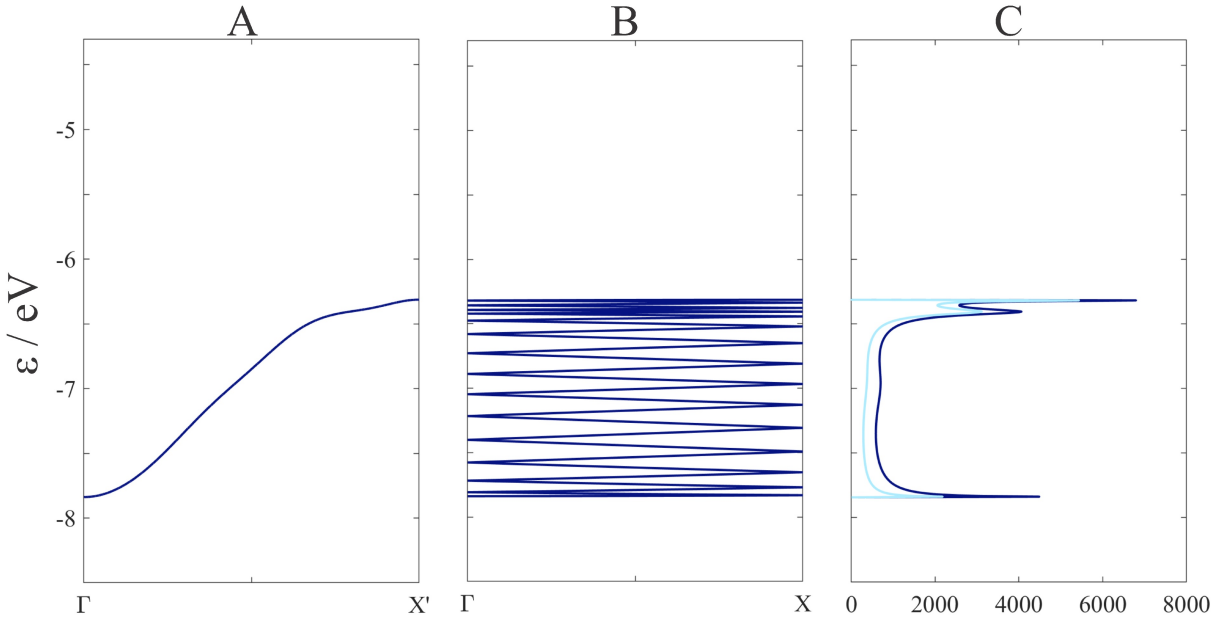

Figure A10. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[50.6]-$(SiMe_2)_\infty$

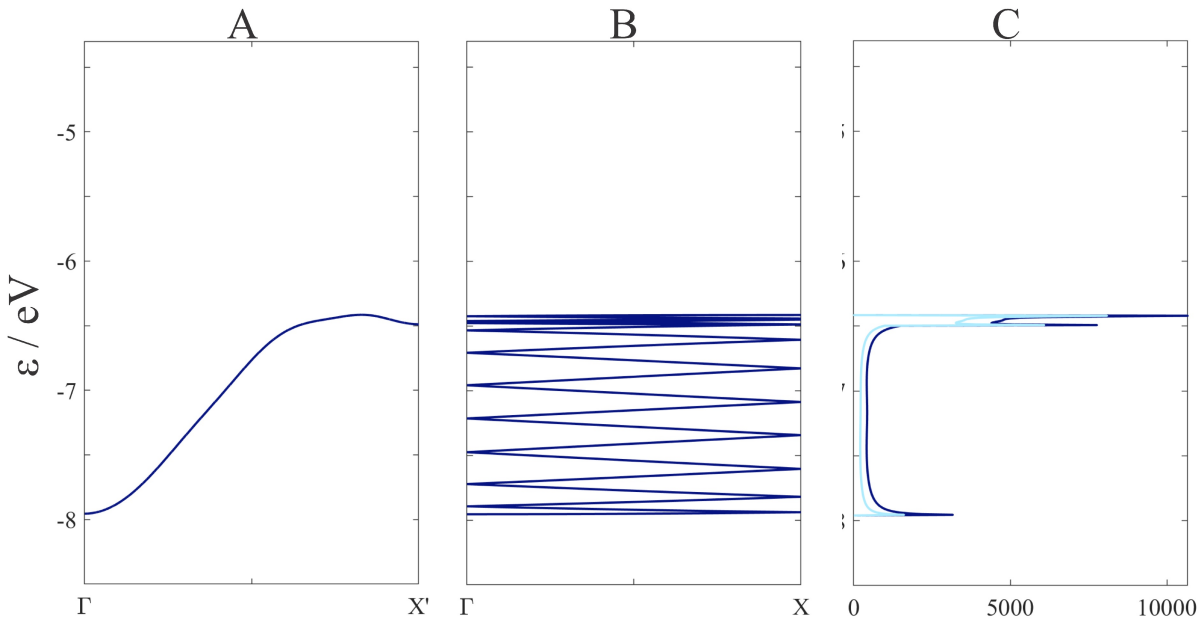

Figure A11. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark blue) and projected Si (light blue) density of states (C) for *all*-[35.9]-$(SiMe_2)_\infty$

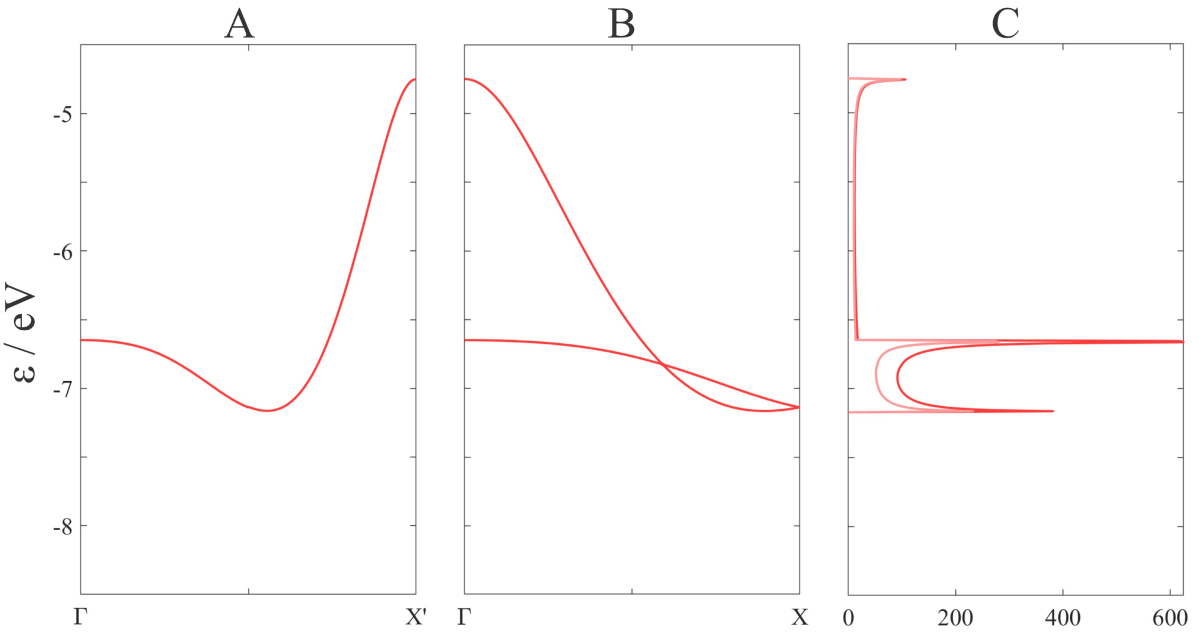

Figure A12. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[180]-$(GeMe_2)_\infty$

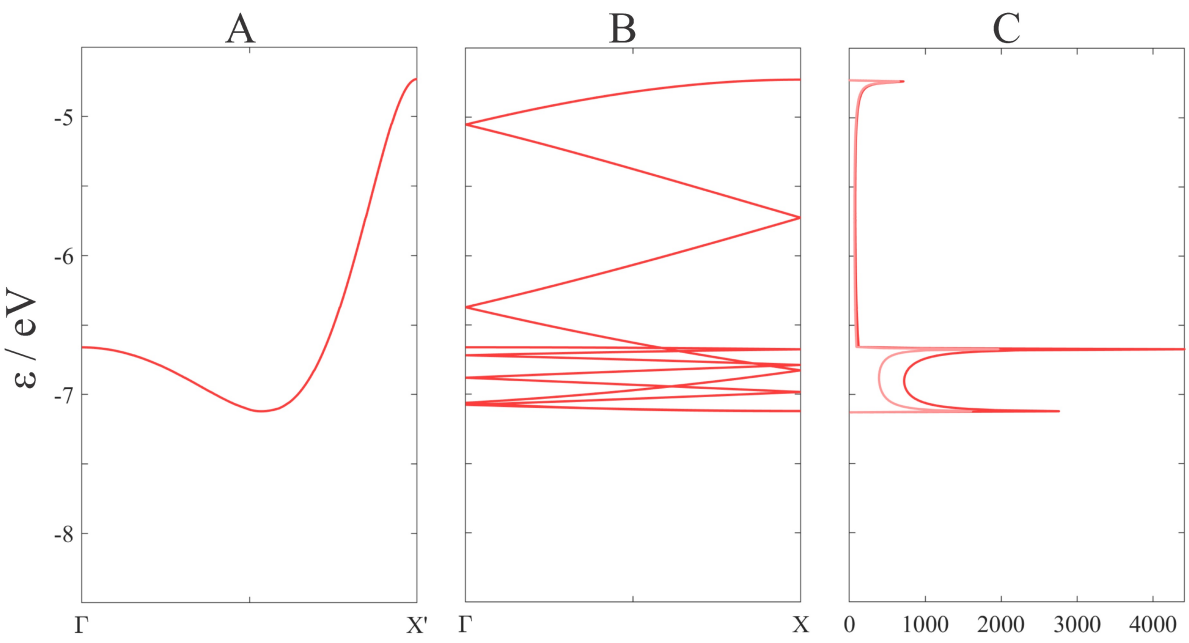

Figure A13. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[163.2]-$(GeMe_2)_\infty$

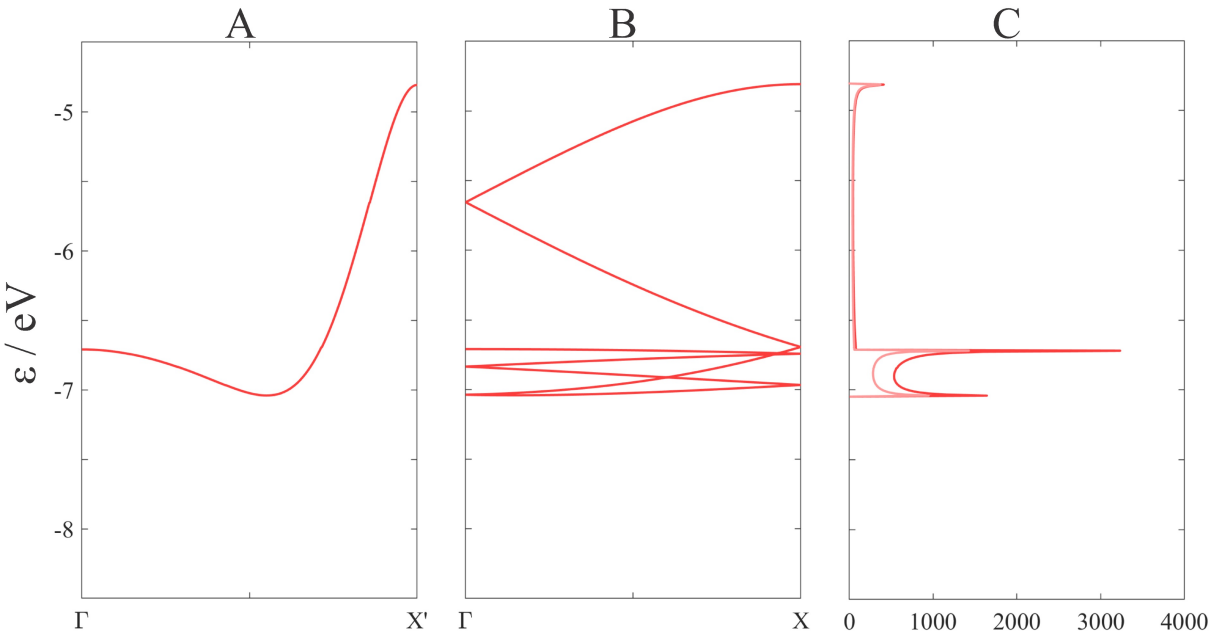

Figure A14. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[149.0]-$(GeMe_2)_\infty$

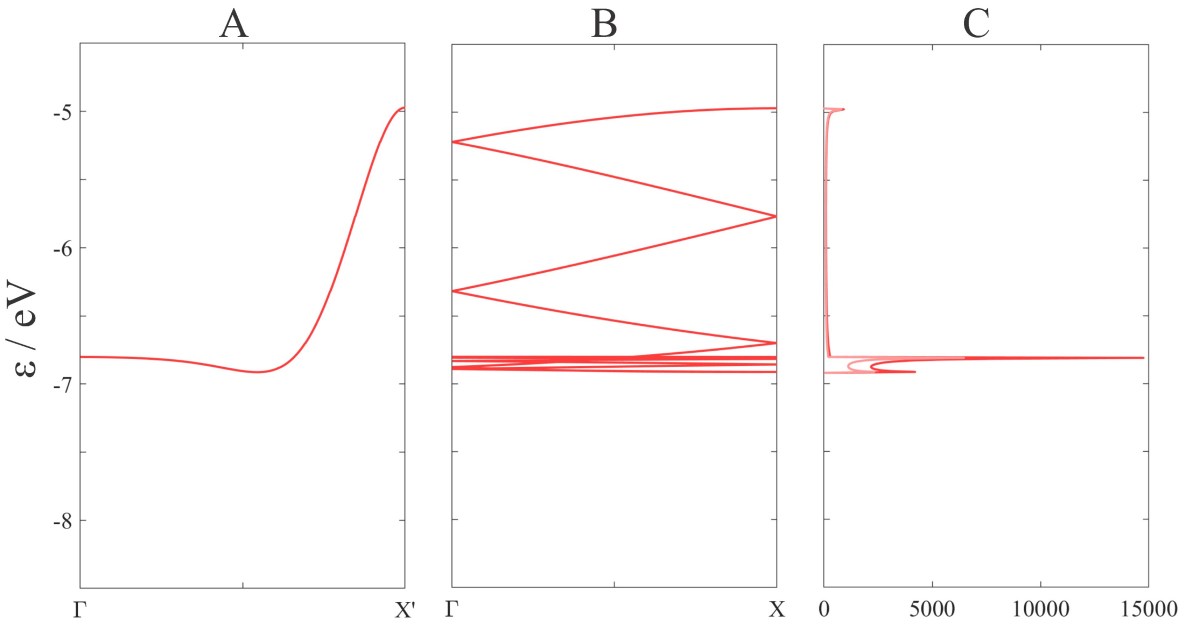

Figure A15. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[130.4]-$(GeMe_2)_\infty$

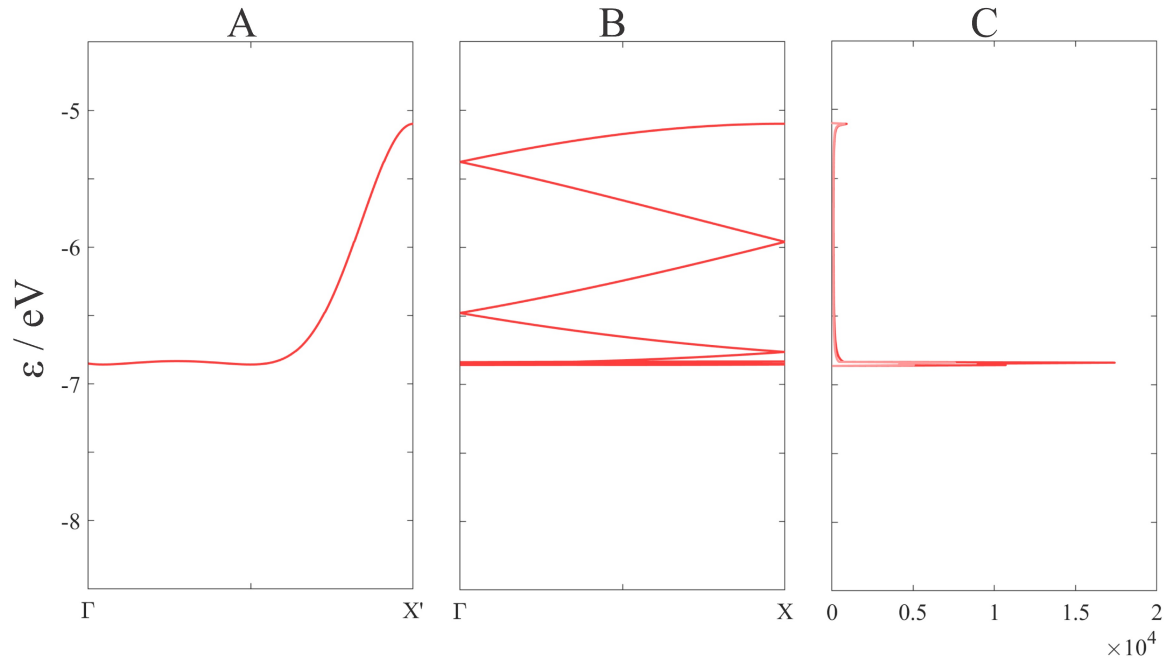

Figure A16. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[121.5]-$(GeMe_2)_\infty$

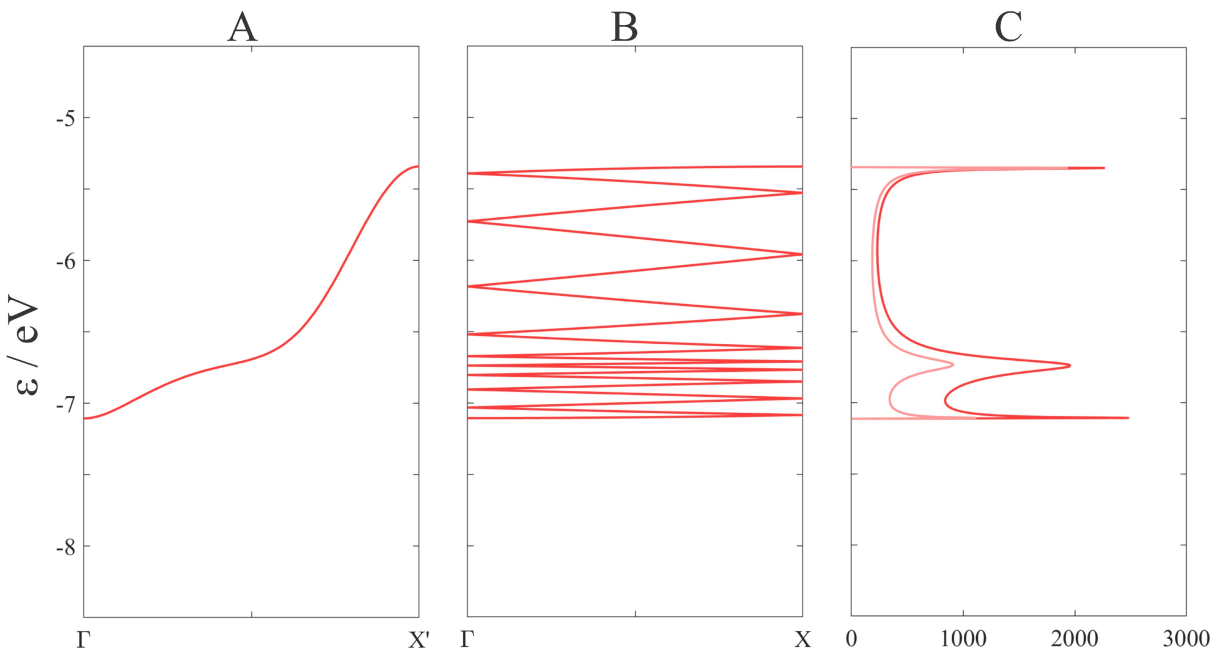

Figure A17. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[-98.4]-$(GeMe_2)_\infty$

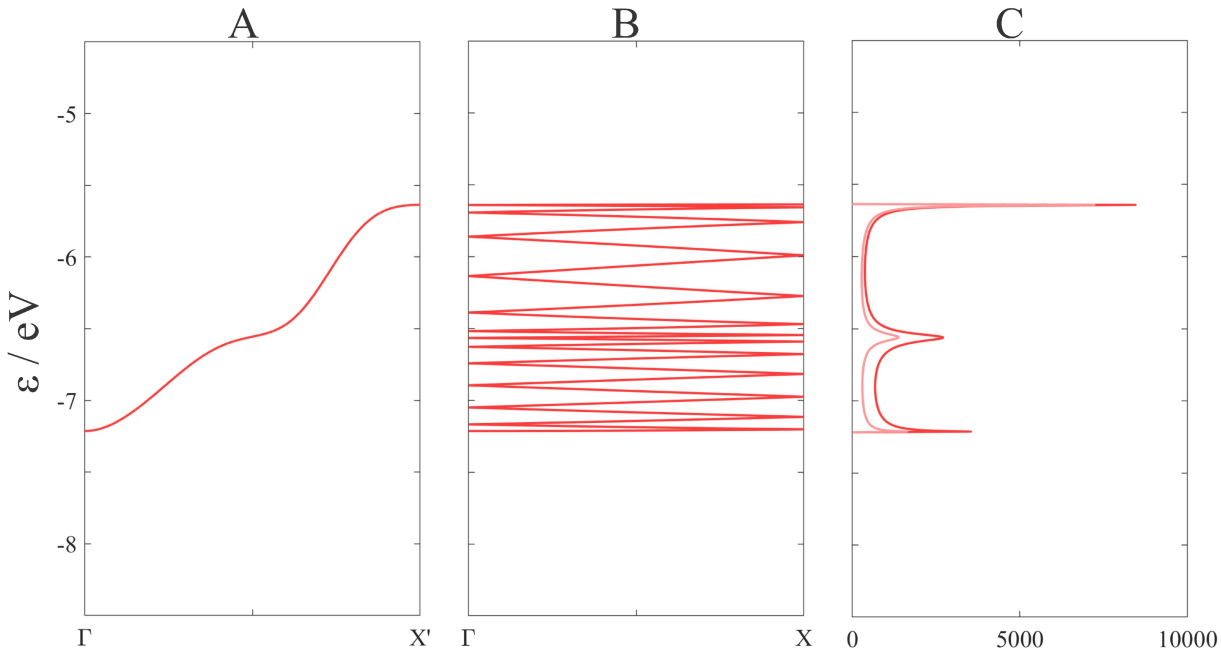

Figure A18. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[86.5]-$(GeMe_2)_\infty$

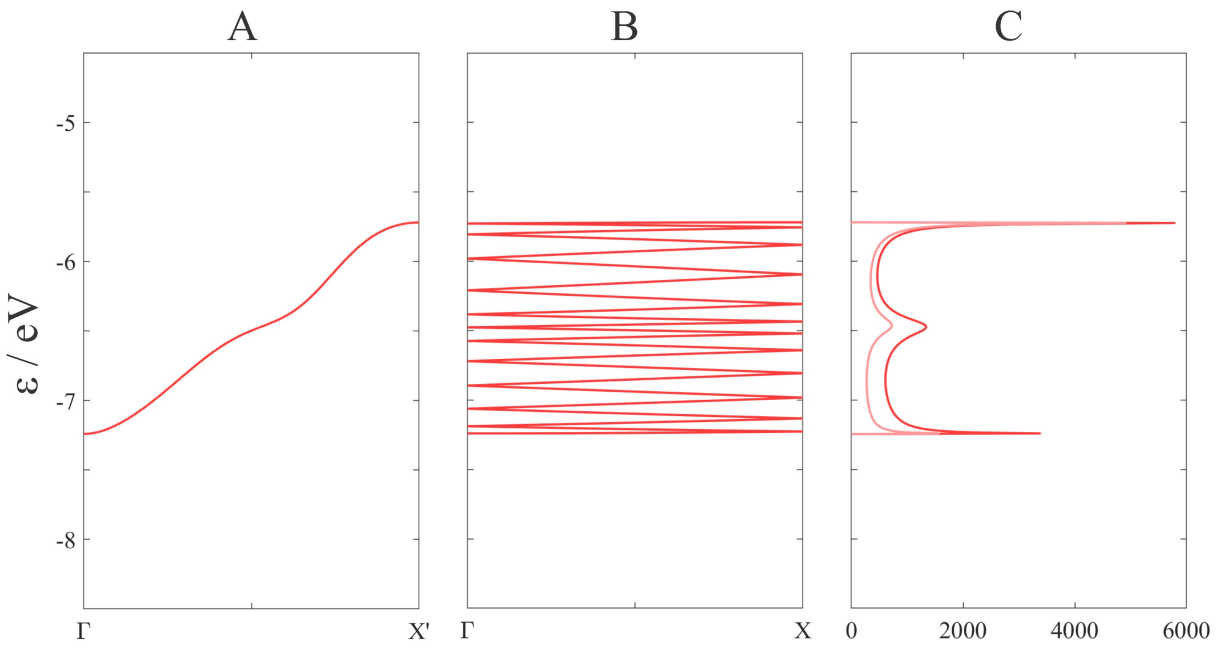

Figure A19. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[-75.3]-$(GeMe_2)_\infty$

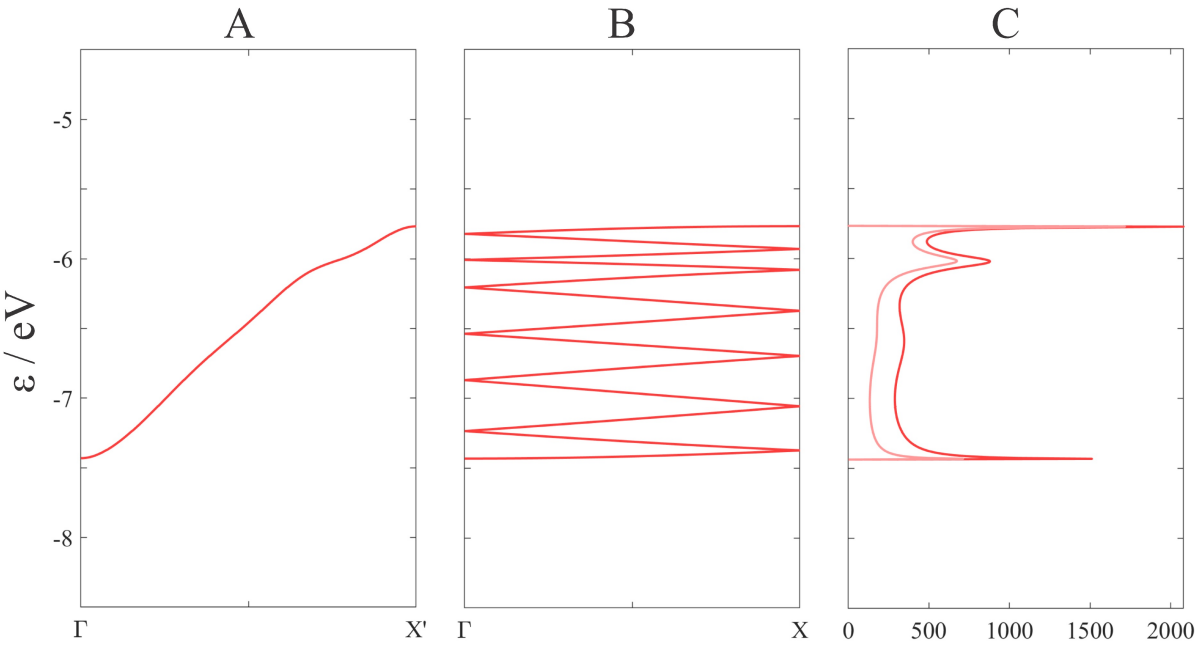

Figure A20. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[60.1]-$(GeMe_2)_\infty$

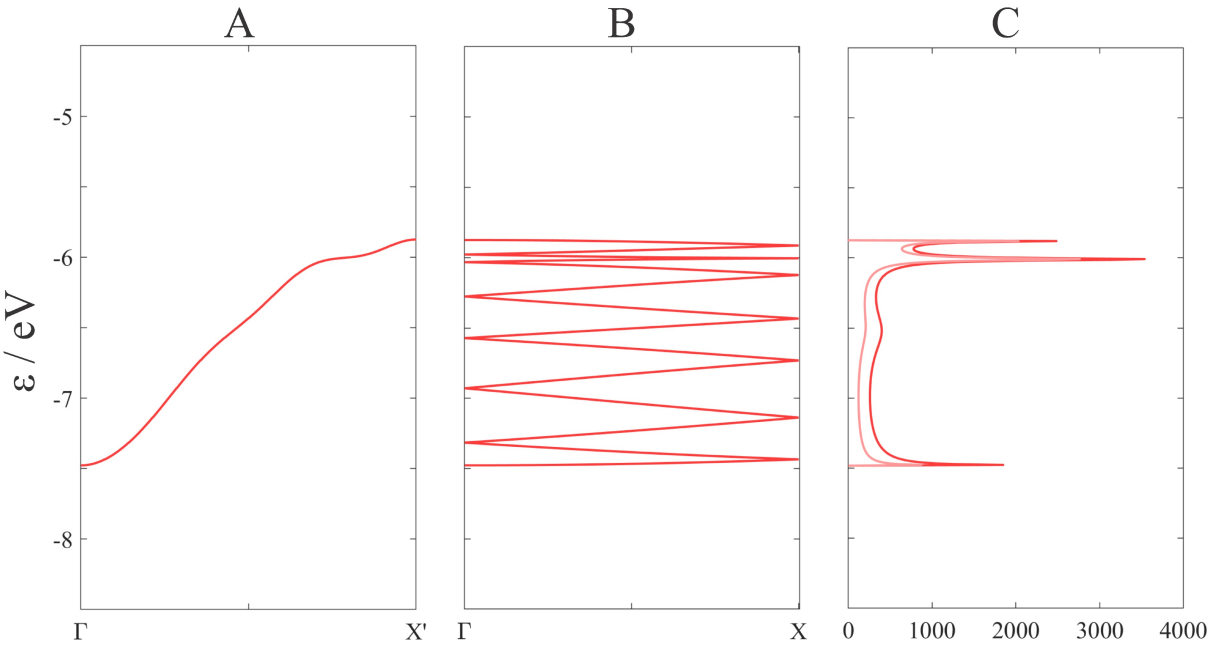

Figure A21. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[-52.5]-$(GeMe_2)_\infty$

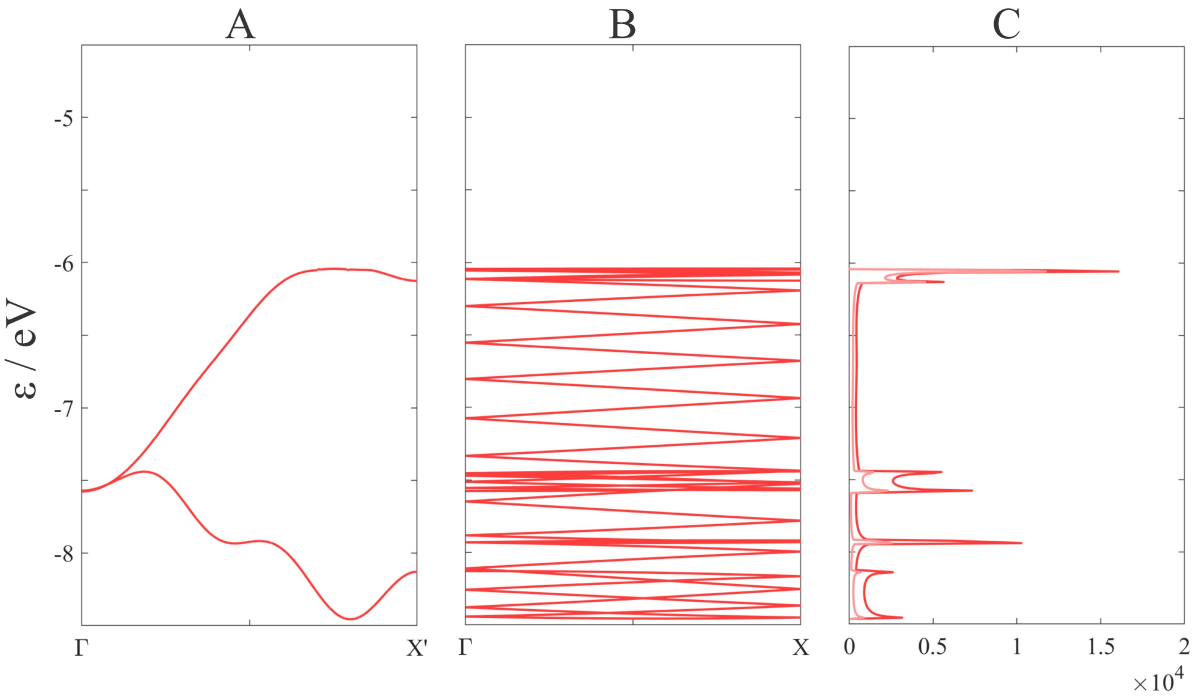

Figure A22. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (red) and projected Ge (light red) density of states (C) for *all*-[-35.5]-$(GeMe_2)_\infty$

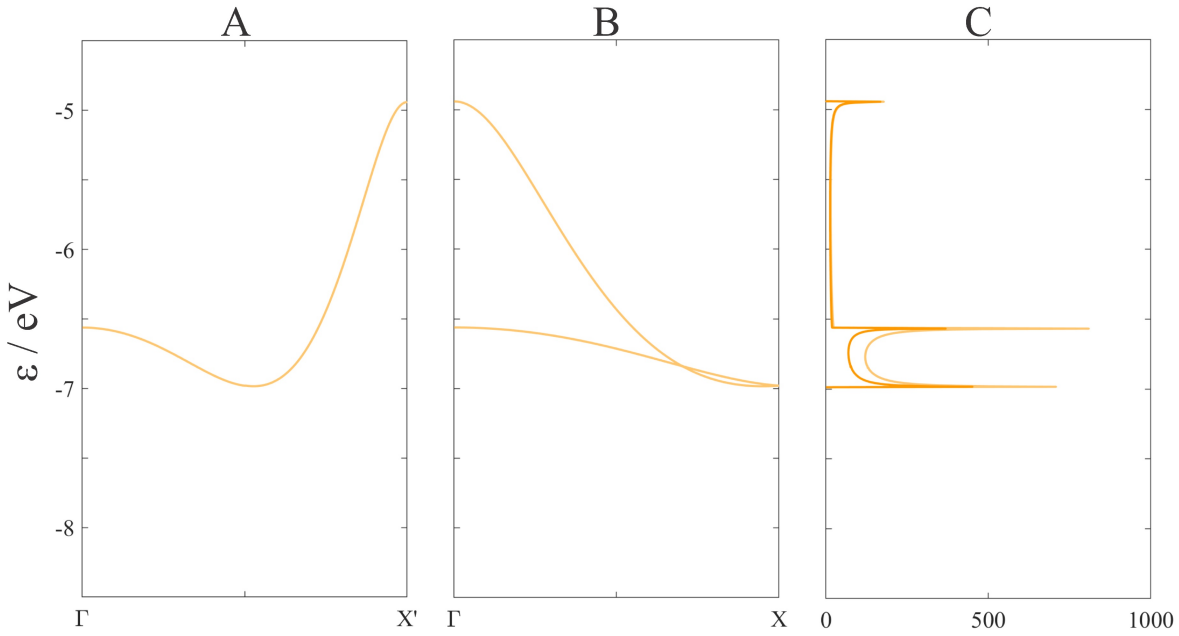

Figure A23. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[180]-$(SnMe_2)_\infty$

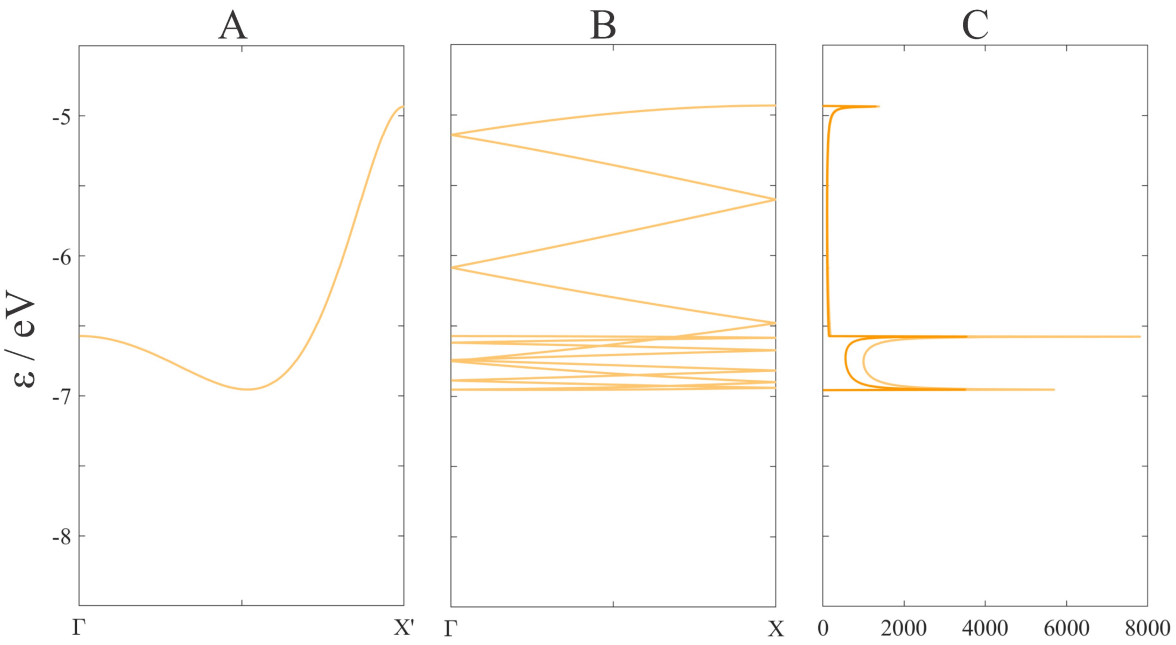

Figure A24. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[165.5]-$(SnMe_2)_\infty$

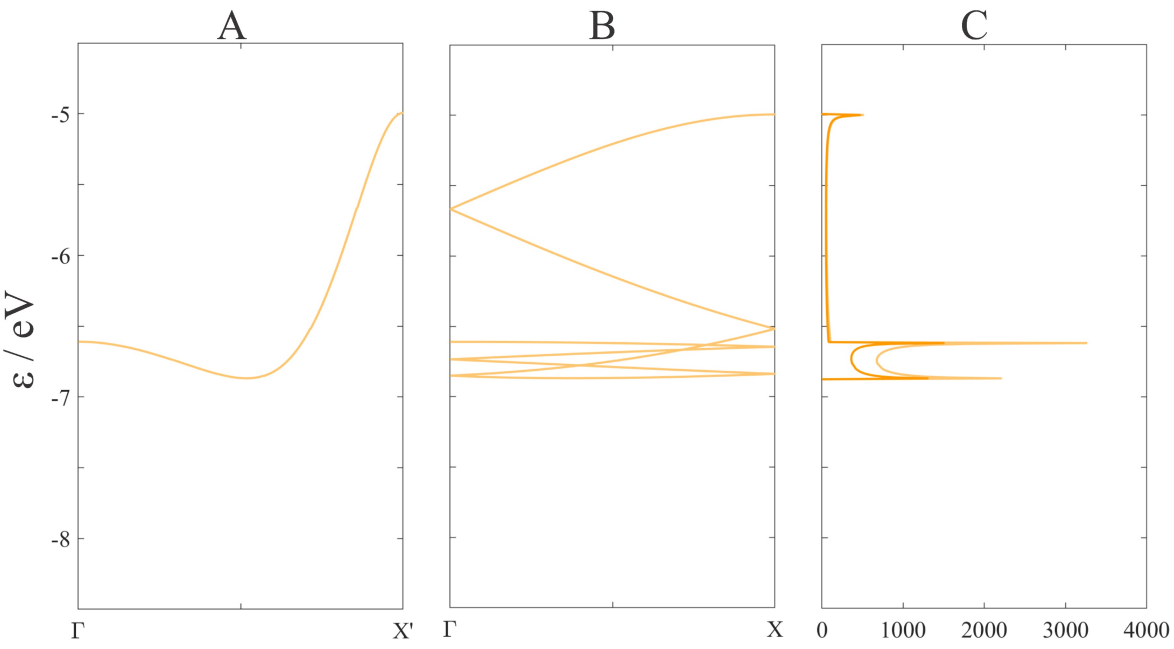

Figure A25. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[148.9]-$(SnMe_2)_\infty$

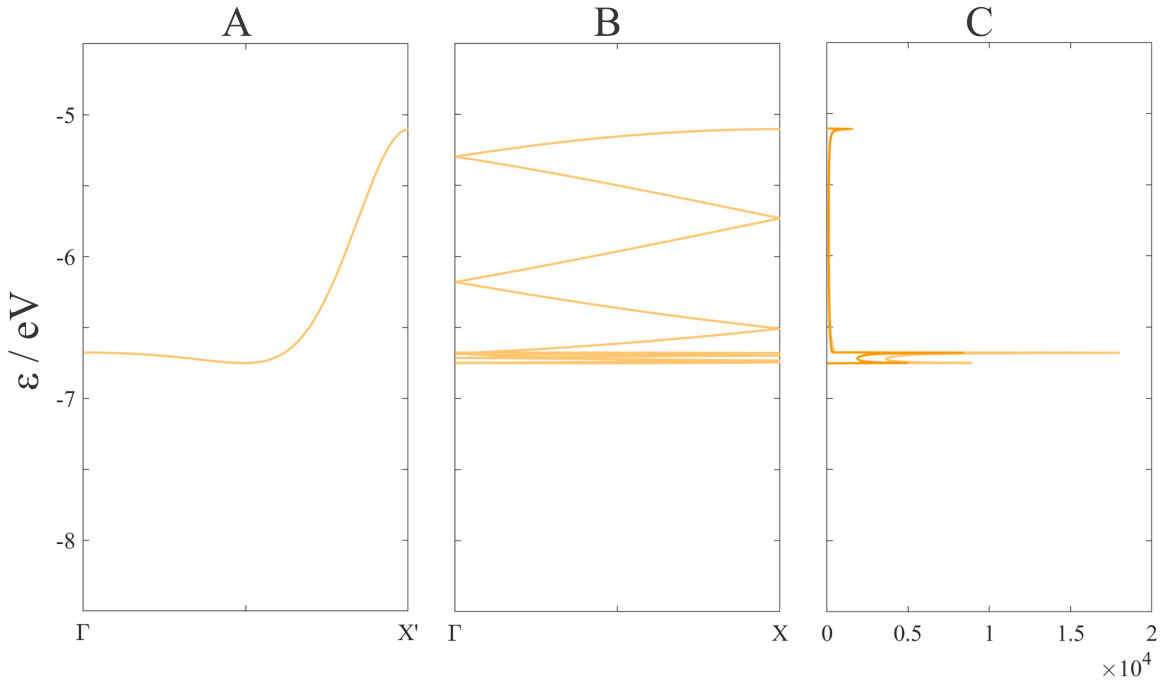

Figure A26. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[129.9]-$(SnMe_2)_\infty$

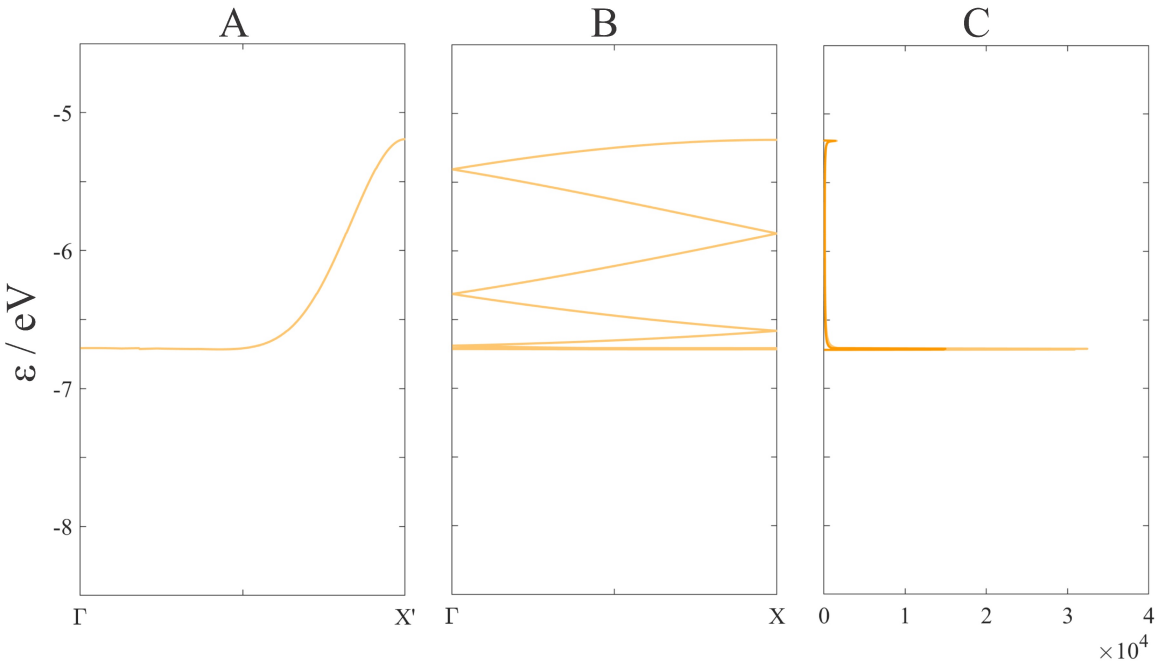

Figure A27. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[-118.8]-$(SnMe_2)_\infty$

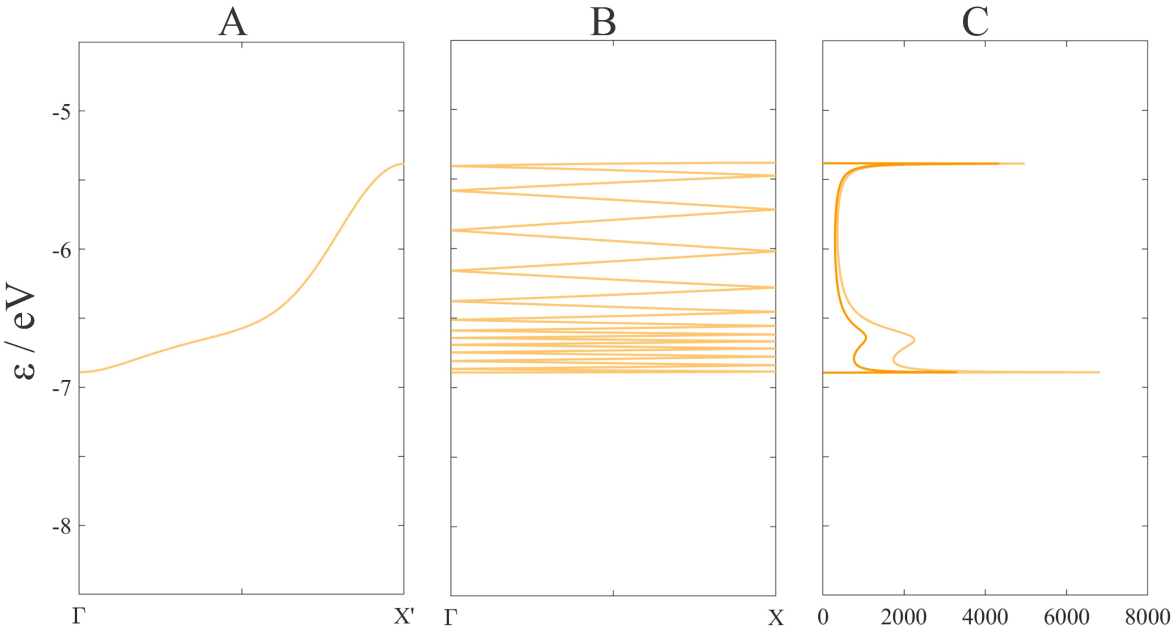

Figure A28. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[-99.7]-$(SnMe_2)_\infty$

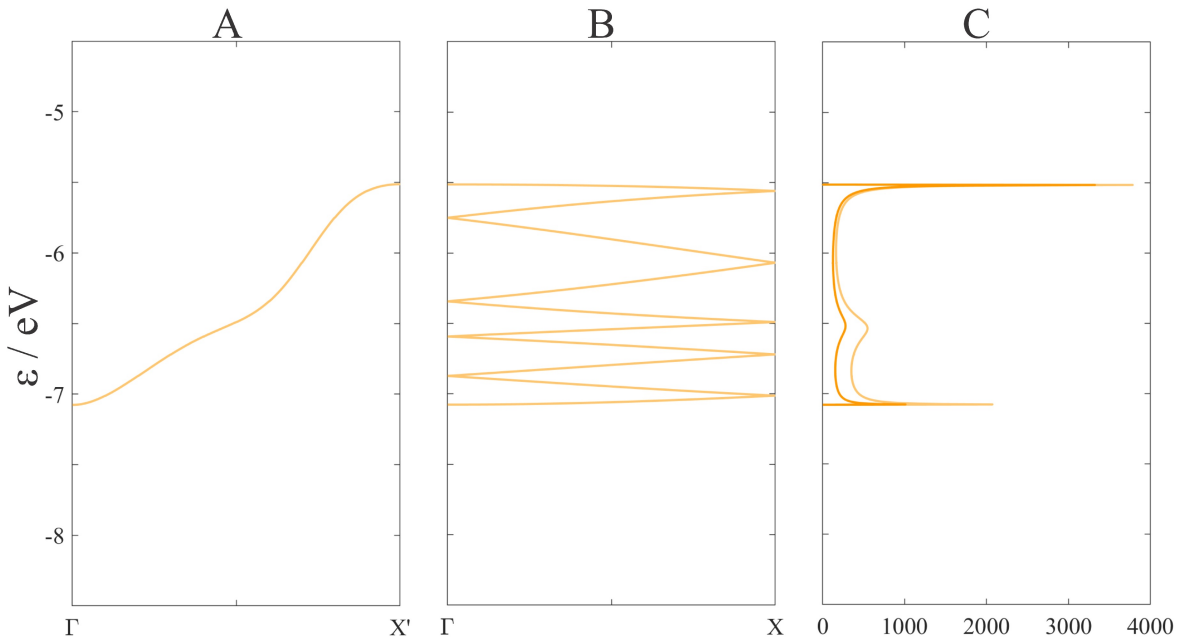

Figure A29. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[87.3]-$(SnMe_2)_\infty$

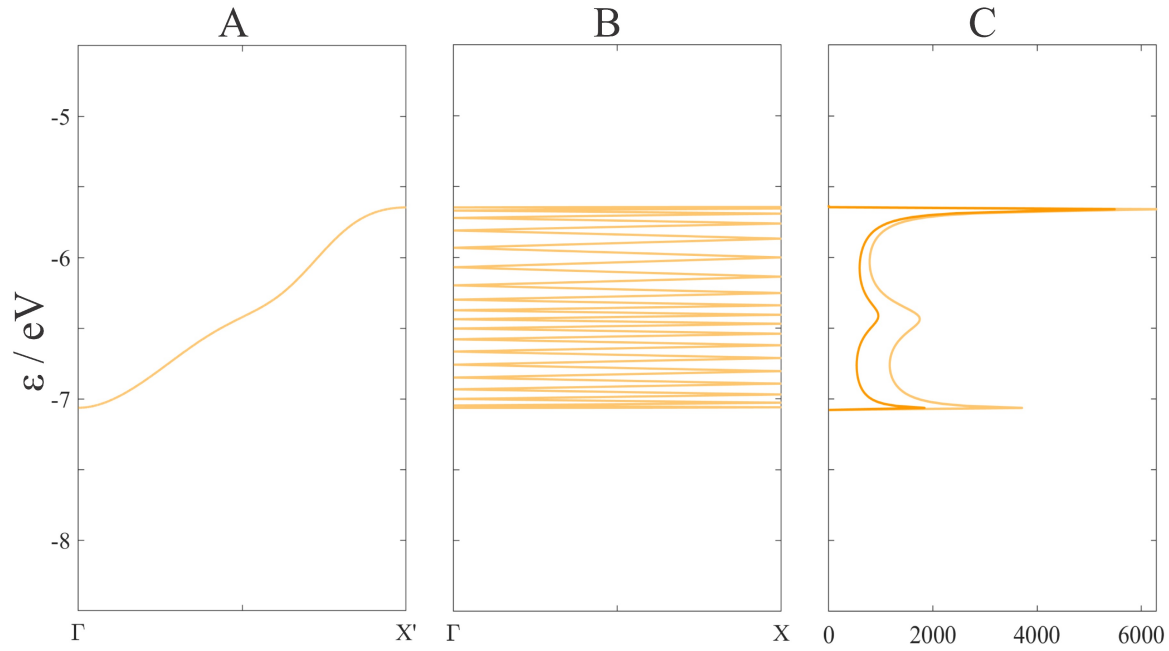

Figure A30. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[-73.6]-$(SnMe_2)_\infty$

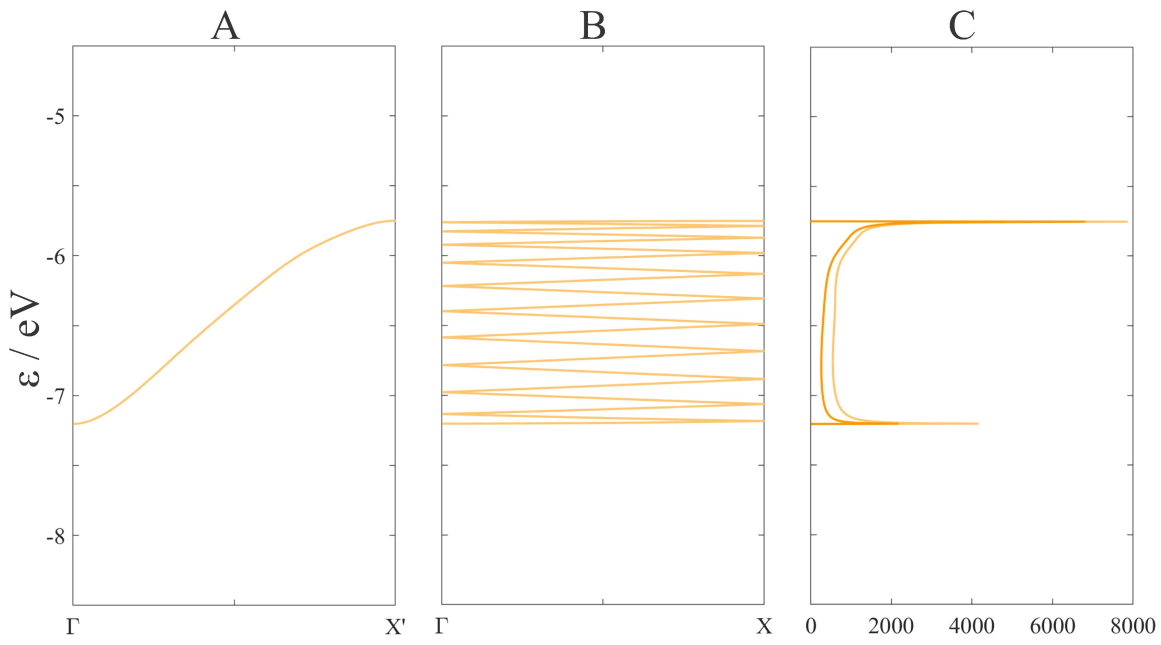

Figure A31. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[60.4]-$(SnMe_2)_\infty$

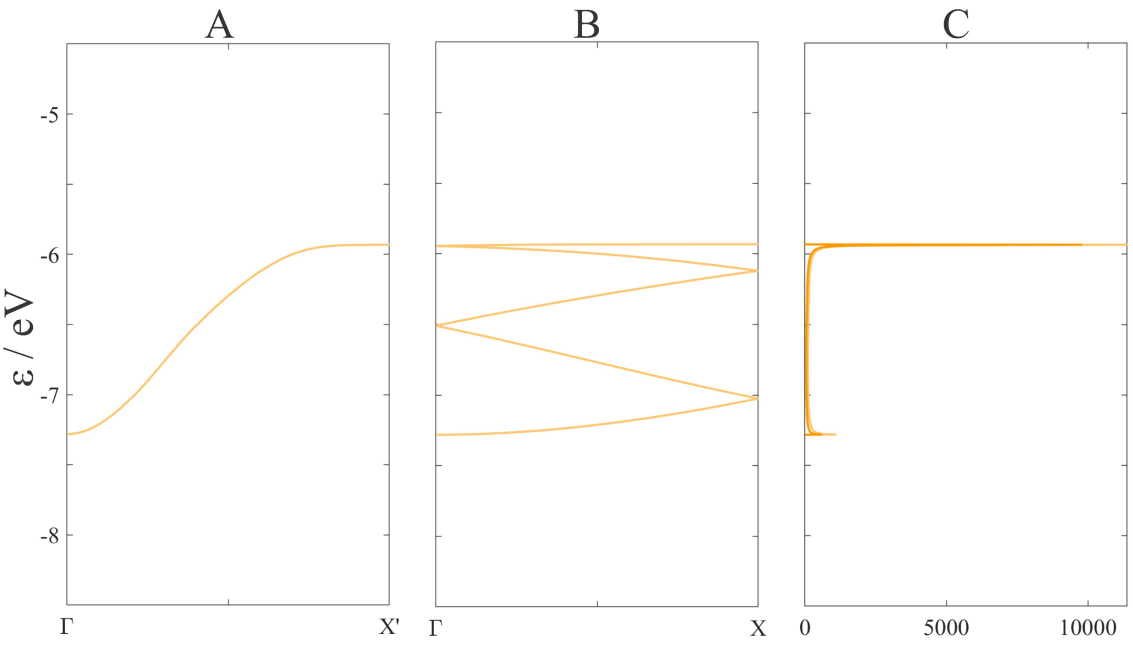

Figure A32. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[43.4]-$(SnMe_2)_\infty$

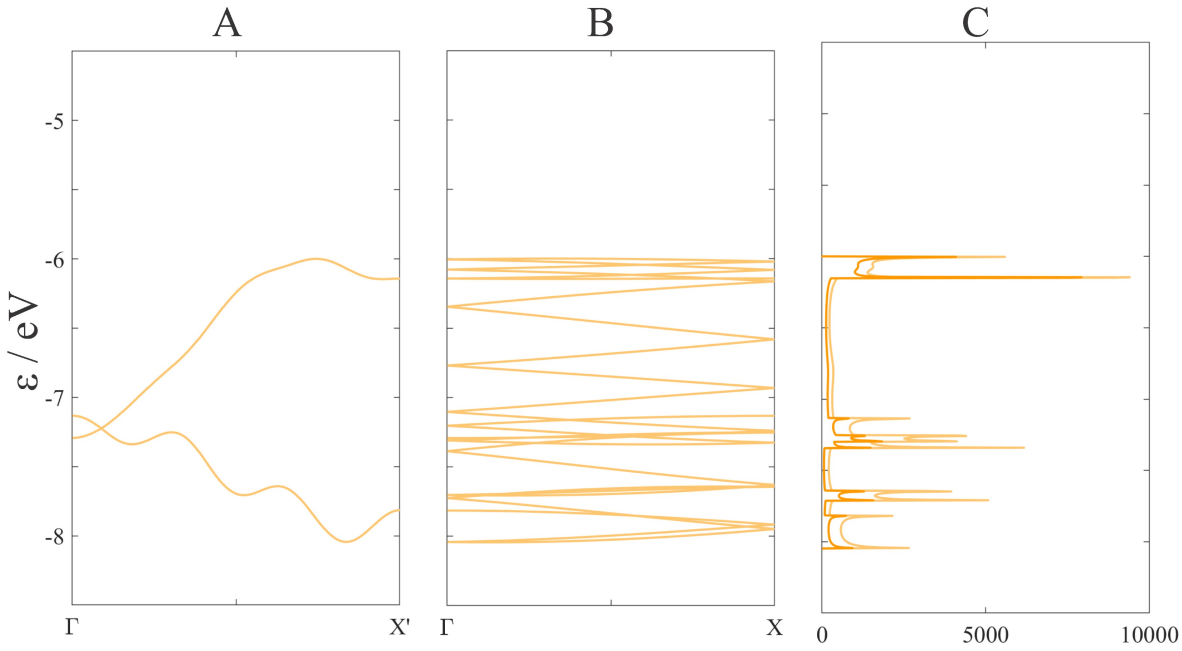

Figure A33. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (light yellow) and projected Sn (dark yellow) density of states (C) for *all*-[24.5]-$(SnMe_2)_\infty$

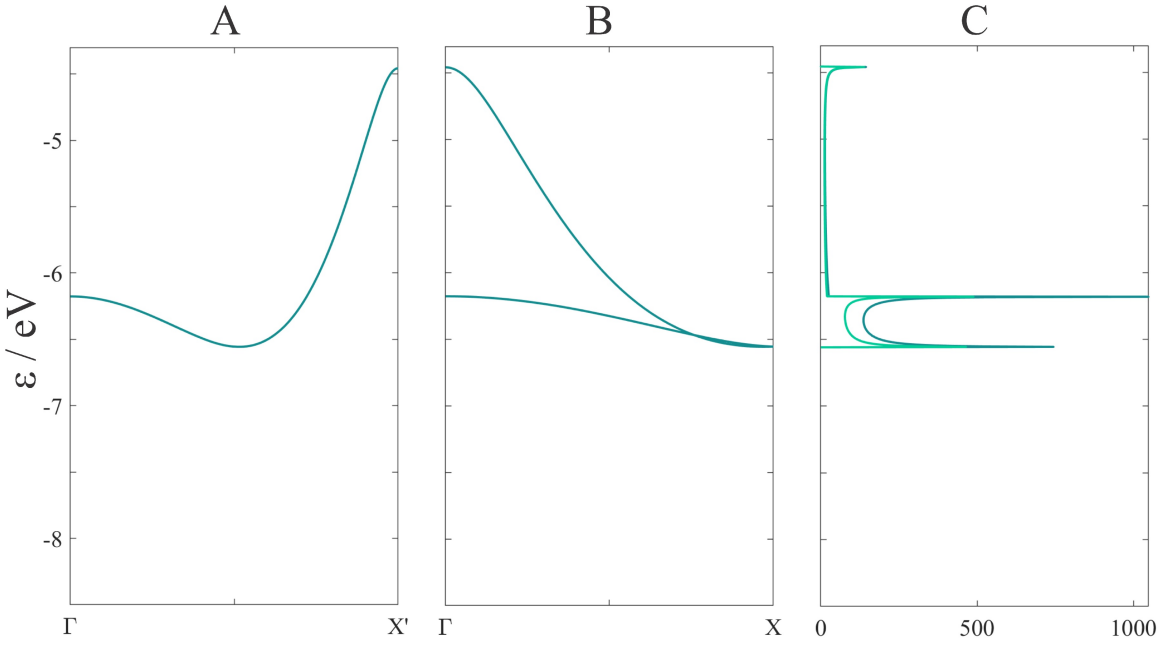

Figure A34. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb light green) density of states (C) for *all*-[180.0]-$(PbMe_2)_\infty$

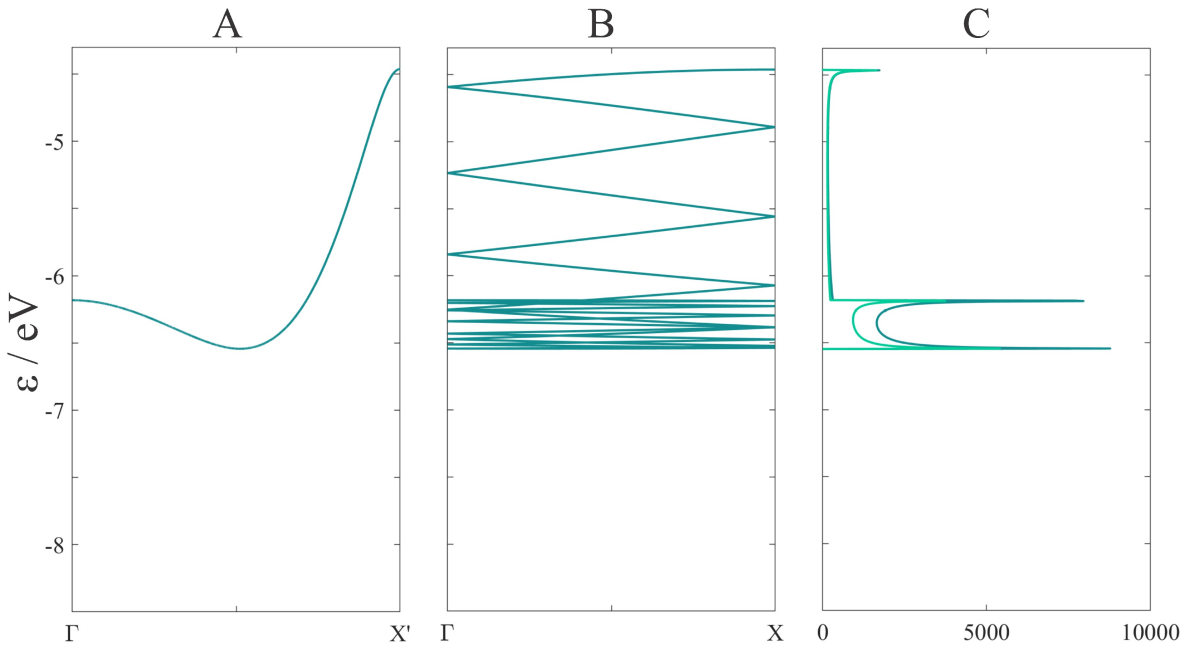

Figure A35. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[170.6]-$(PbMe_2)_\infty$

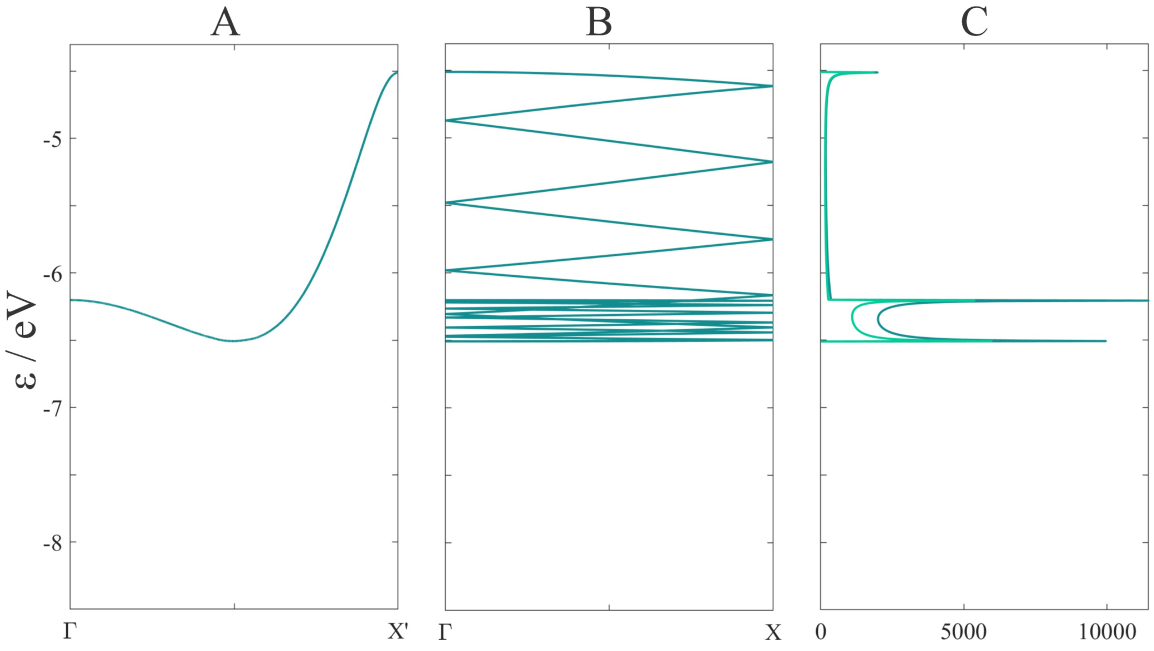

Figure A36. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[161.9]-$(PbMe_2)_\infty$

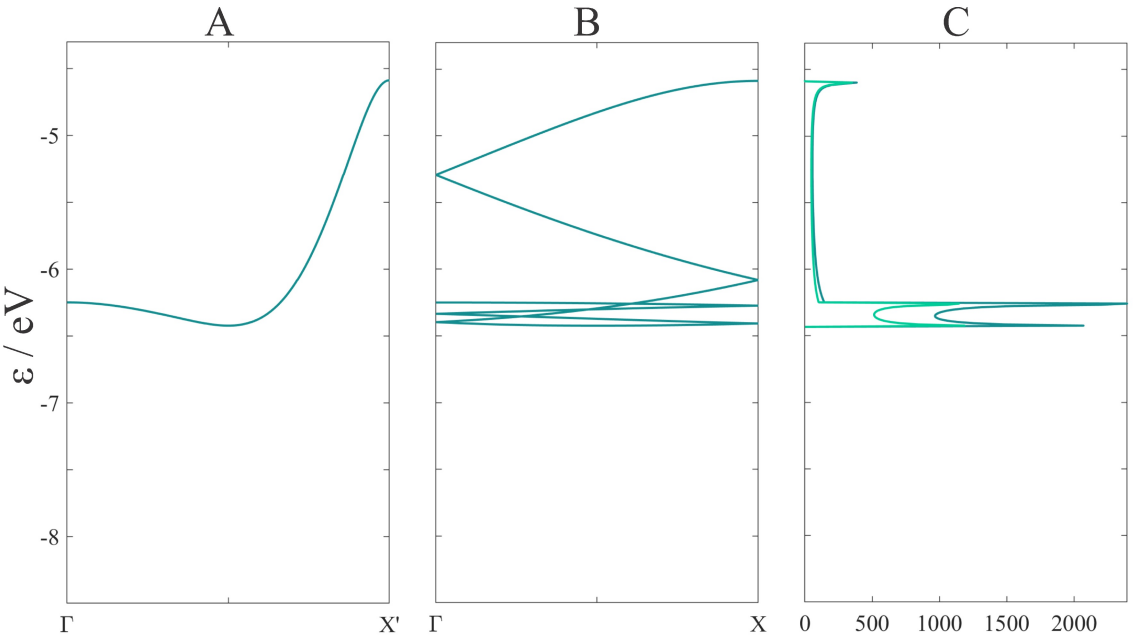

Figure A37. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[148.7]-$(PbMe_2)_\infty$

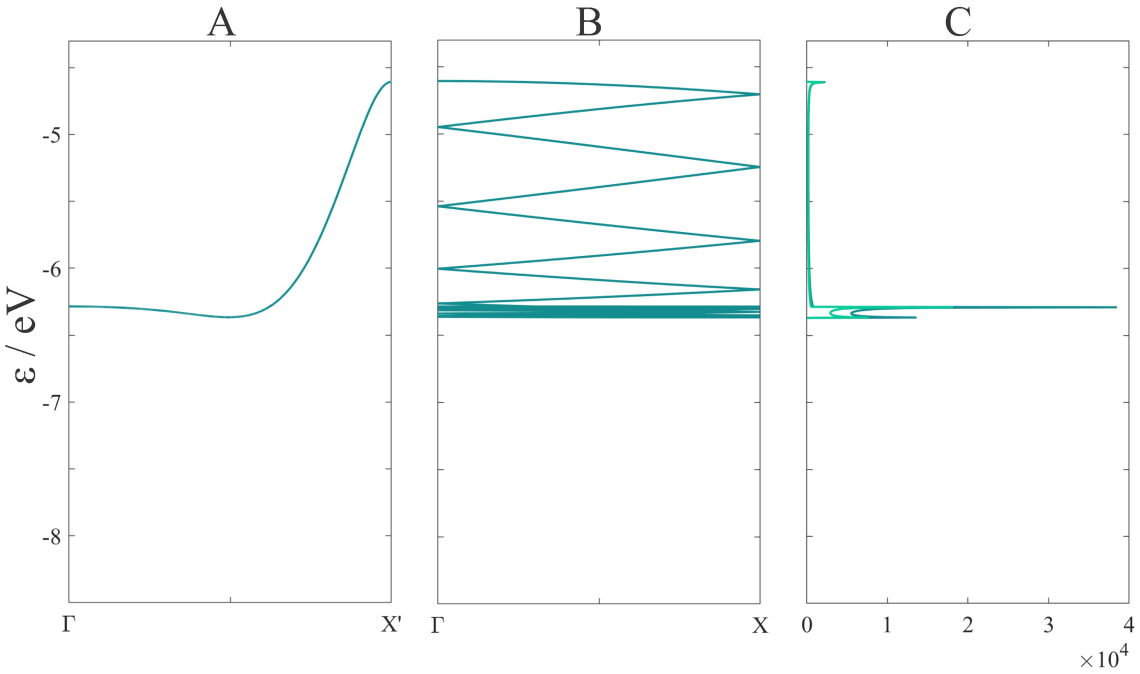

Figure A38. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[140.1]-$(PbMe_2)_\infty$

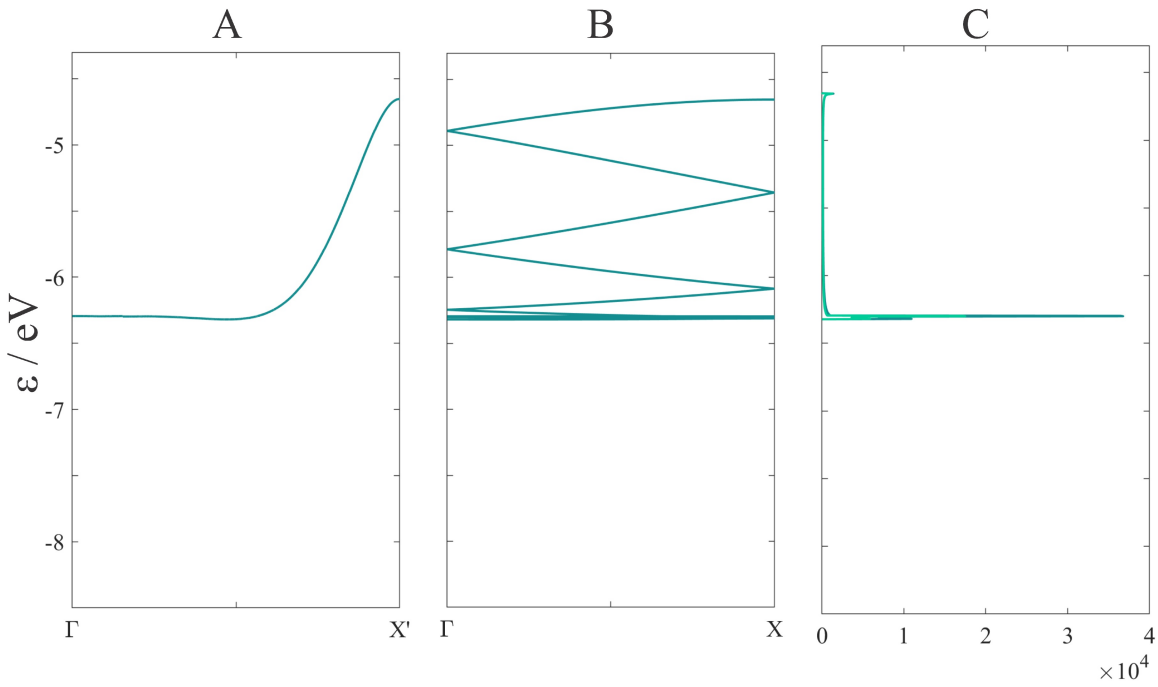

Figure A39. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[-129.8]-$(PbMe_2)_\infty$

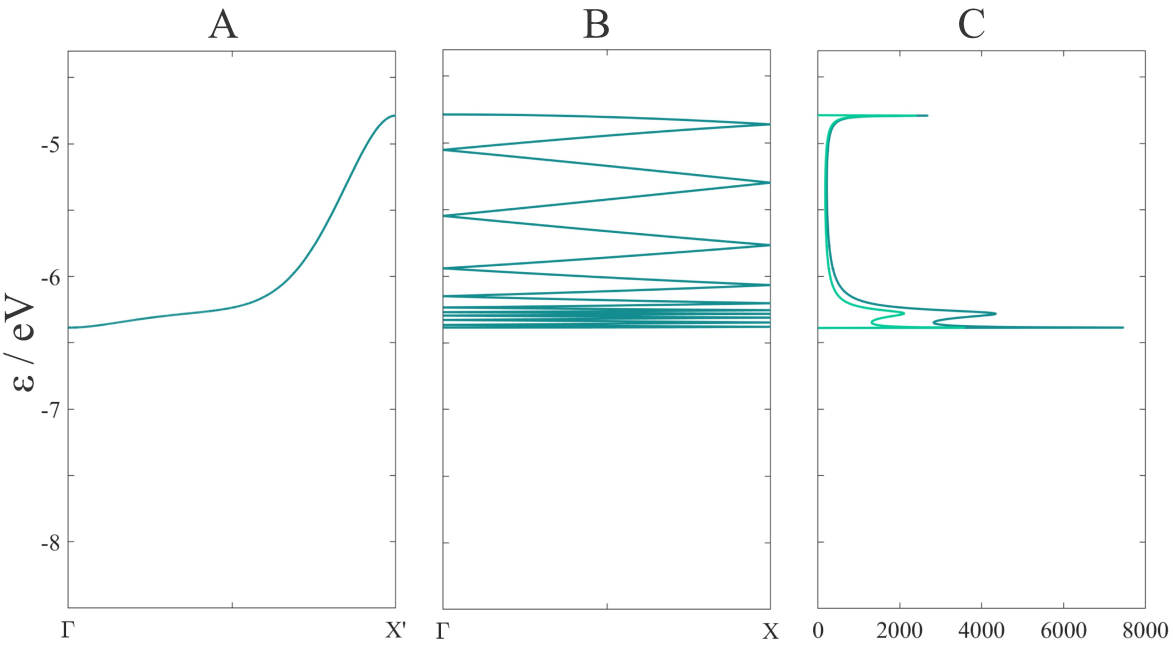

Figure A40. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[-113.9]-$(PbMe_2)_\infty$

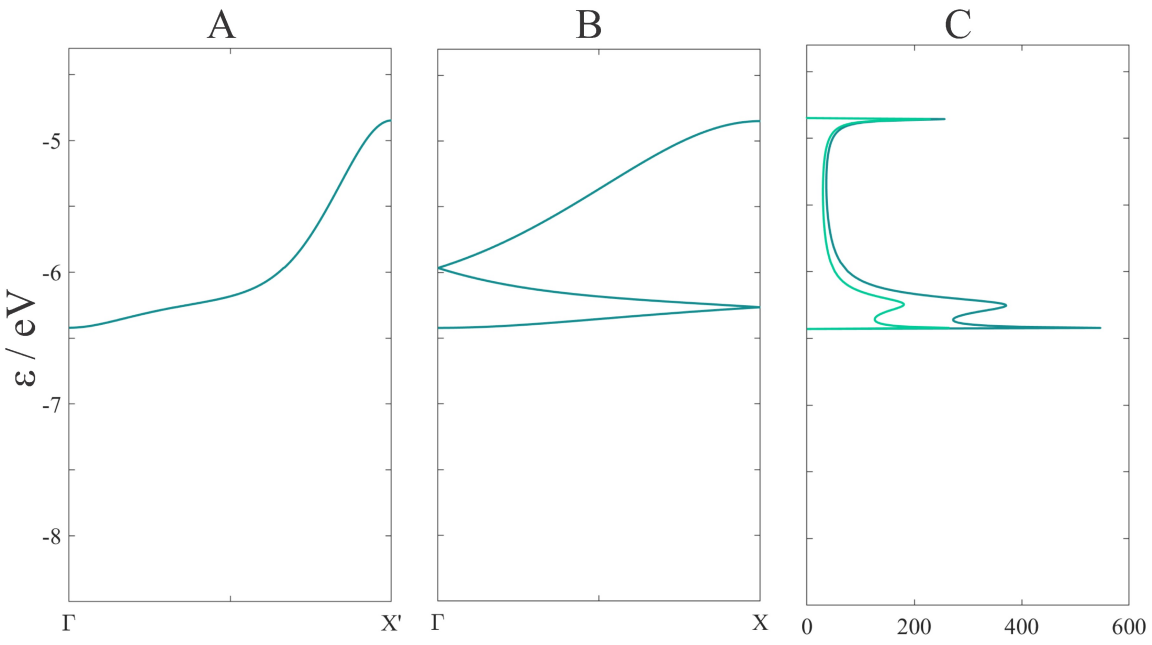

Figure A41. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[106.2]-$(PbMe_2)_\infty$

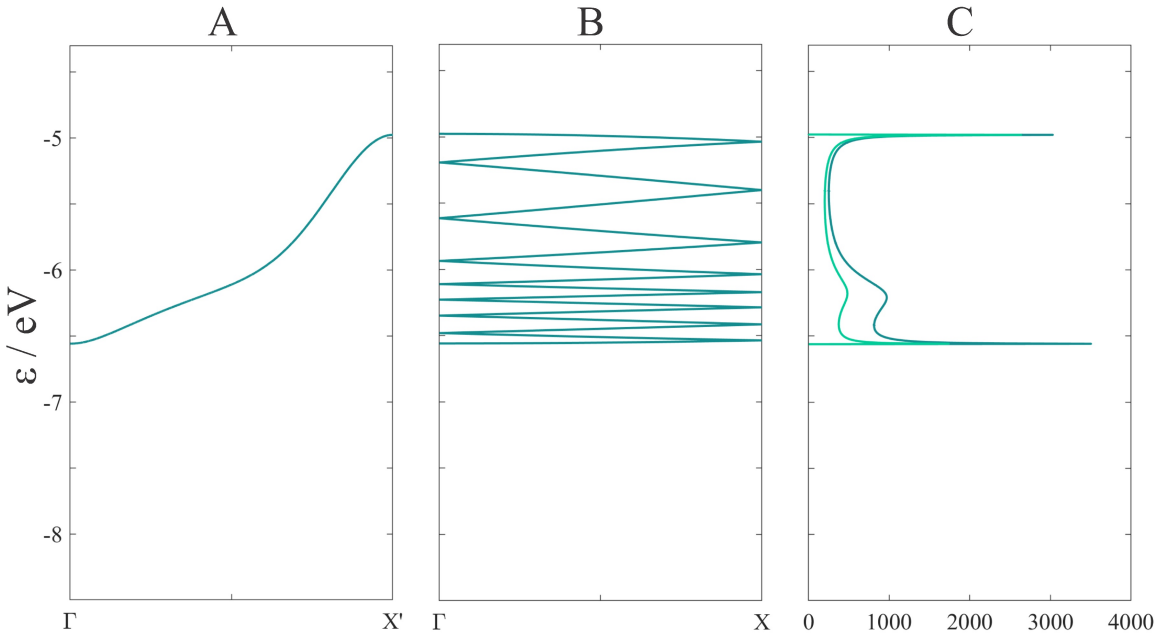

Figure A42. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[-93.9]-$(PbMe_2)_\infty$

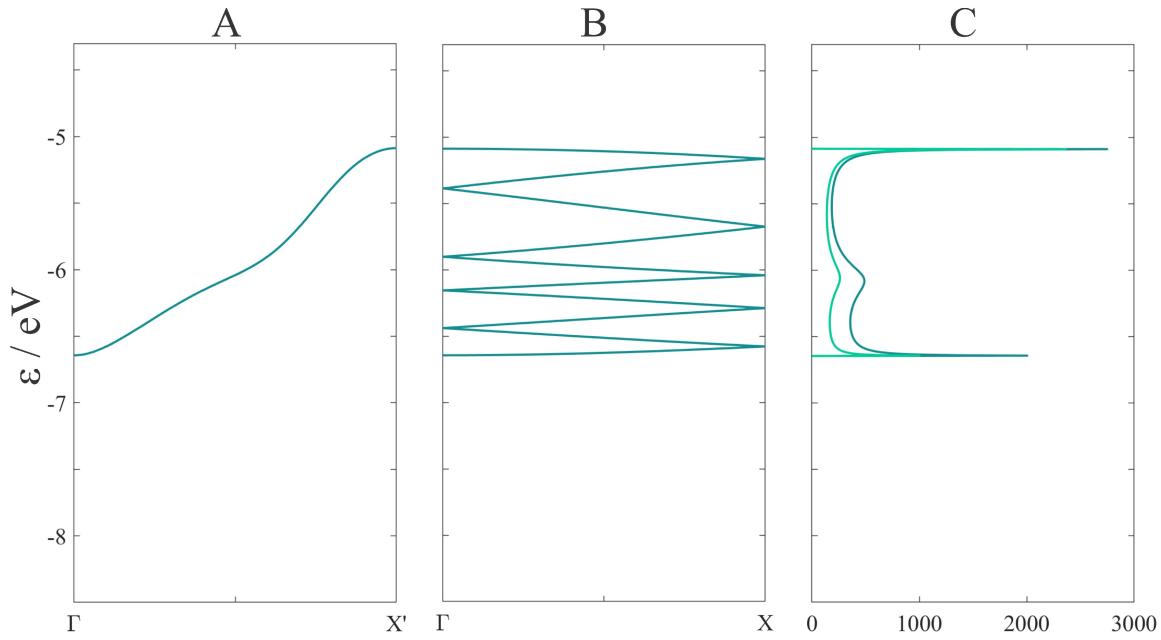

Figure A43. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[-85.3]-$(PbMe_2)_\infty$

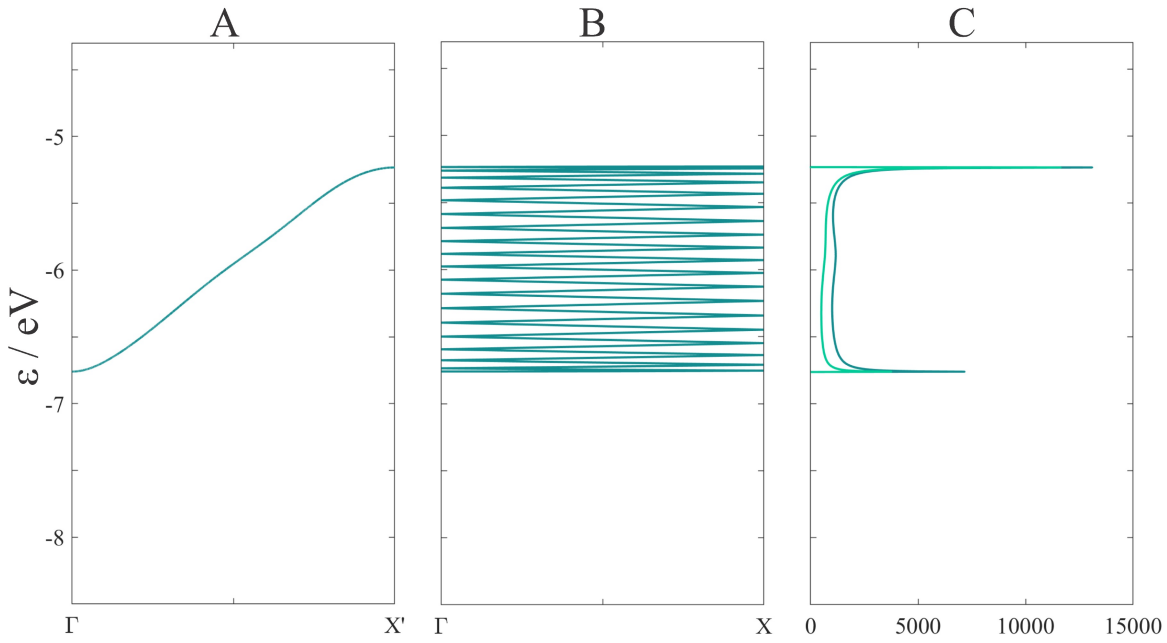

Figure A44. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[61.1]-$(PbMe_2)_\infty$

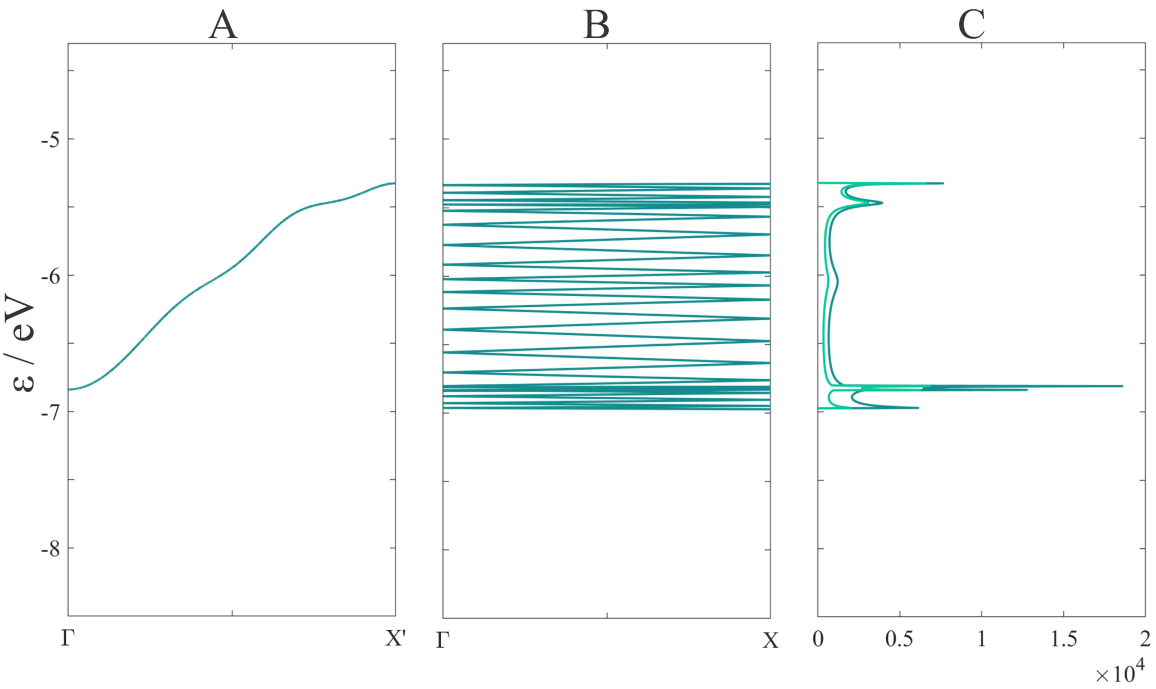

Figure A45. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[-50.4]-$(PbMe_2)_\infty$

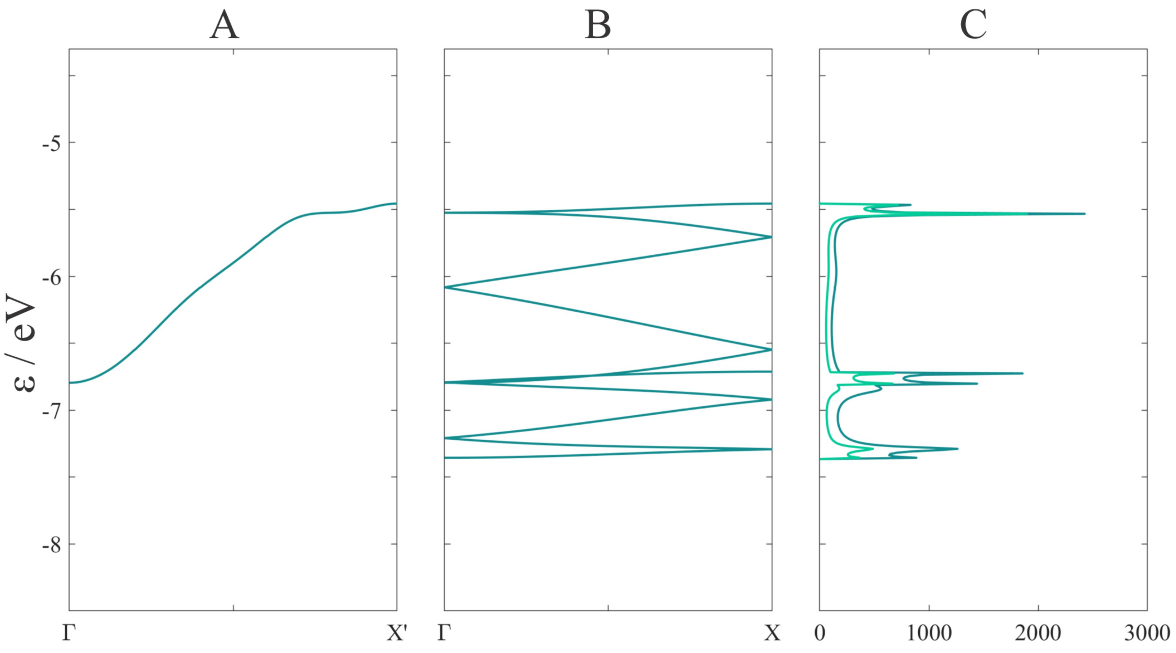

Figure A46. DFT band structure plotted in the Jones zone (A) and the first Brillouin zone (B) and total (dark green) and projected Pb (light green) density of states (C) for *all*-[38.4]-$(PbMe_2)_\infty$

Optimized geometries

MP2/6311G optimized geometry, all-*anti*-Si_4Me_{10}**

44
RI-MP2
Energy= -1554.06541759012339
TD B3LYP
Energy= -1557.45856054

C	-1.757772	1.025254	1.540012
Si	-0.644942	0.985011	0.000000
C	-1.757772	1.025254	-1.540012
Si	0.644942	-0.985011	0.000000
C	1.757772	-1.025254	-1.540012
Si	-0.663963	-2.944515	0.000000
C	-1.757772	-3.042374	1.537536
C	1.757772	-1.025254	1.540012
Si	0.663963	2.944515	0.000000
C	1.757772	3.042374	1.537536
C	0.497688	-4.437819	0.000000
C	-1.757772	-3.042374	-1.537536
C	-0.497688	4.437819	0.000000
C	1.757772	3.042374	-1.537536
H	-2.345910	1.949290	1.574273
H	-2.461587	0.186361	1.548017
H	-1.169775	0.972539	2.462504
H	-2.345910	1.949290	-1.574273
H	-1.169775	0.972539	-2.462504
H	-2.461587	0.186361	-1.548017
H	2.345910	-1.949290	1.574273
H	2.461587	-0.186361	1.548017
H	1.169775	-0.972539	2.462504
H	2.345910	-1.949290	-1.574273
H	1.169775	-0.972539	-2.462504
H	2.461587	-0.186361	-1.548017
H	1.144195	-4.444740	-0.883930
H	-0.071507	-5.374819	0.000000
H	1.144195	-4.444740	0.883930
H	-1.166722	-2.966727	-2.456418
H	-2.296180	-3.996849	-1.568957
H	-2.503689	-2.241547	-1.556673
H	-2.296180	-3.996849	1.568957
H	-1.166722	-2.966727	2.456418
H	-2.503689	-2.241547	1.556673
H	-1.144195	4.444740	-0.883930

H	0.071507	5.374819	0.000000
H	-1.144195	4.444740	0.883930
H	1.166722	2.966727	-2.456418
H	2.296180	3.996849	-1.568957
H	2.503689	2.241547	-1.556673
H	2.296180	3.996849	1.568957
H	1.166722	2.966727	2.456418
H	2.503689	2.241547	1.556673

MP2/6311G optimized geometry, all-*transoid*-Si_4Me_{10}**

44
RI-MP2
Energy= -1554.06689167058721
TD B3LYP
Energy= -1557.45865421

Si	-0.705971	0.941272	-0.188243
Si	0.705971	-0.941272	-0.188243
Si	0.525825	2.916790	0.153917
C	2.024226	-0.798352	1.173529
C	1.591473	-1.036305	-1.866584
Si	-0.525825	-2.916790	0.153917
C	-2.024226	0.798352	1.173529
C	-1.591473	1.036305	-1.866584
C	-0.548402	4.420349	-0.248060
C	2.052379	2.953192	-0.960368
C	1.079311	3.035580	1.956648
C	0.548402	-4.420349	-0.248060
C	-2.052379	-2.953192	-0.960368
C	-1.079311	-3.035580	1.956648
H	2.651619	-1.696364	1.210027
H	2.686193	0.056666	0.996683
H	1.571771	-0.670527	2.162692
H	2.287032	-1.882435	-1.895335
H	0.878384	-1.164677	-2.687805
H	2.167234	-0.126213	-2.066926
H	-2.651619	1.696364	1.210027
H	-2.686193	-0.056666	0.996683
H	-1.571771	0.670527	2.162692
H	-2.287032	1.882435	-1.895335
H	-0.878384	1.164677	-2.687805
H	-2.167234	0.126213	-2.066926
H	-0.864043	4.417797	-1.296623
H	0.000000	5.352586	-0.069129
H	-1.452154	4.445429	0.370249
H	1.782518	2.856513	-2.017548
H	2.597886	3.897045	-0.844132
H	2.745785	2.140530	-0.718872
H	1.647395	3.956959	2.130110
H	0.220848	3.044391	2.636674
H	1.718273	2.192989	2.239514
H	0.864043	-4.417797	-1.296623
H	0.000000	-5.352586	-0.069129
H	1.452154	-4.445429	0.370249

H	-1.782518	-2.856513	-2.017548
H	-2.597886	-3.897045	-0.844132
H	-2.745785	-2.140530	-0.718872
H	-1.647395	-3.956959	2.130110
H	-0.220848	-3.044391	2.636674
H	-1.718273	-2.192989	2.239514

MP2/6311G optimized geometry, all-*deviant*- Si_4Me_{10}**

44
RI-MP2
Energy= -1554.06403678244124
TD B3LYP
Energy= -1557.45597774

Si	-0.798847	0.870572	-0.325398
Si	0.798847	-0.870572	-0.325398
Si	0.183660	2.930107	0.261524
C	2.210586	-0.527330	0.912213
C	1.568407	-0.981778	-2.066350
Si	-0.183660	-2.930107	0.261524
C	-2.210586	0.527330	0.912213
C	-1.568407	0.981778	-2.066350
C	-1.071779	4.332334	0.014345
C	1.699295	3.284559	-0.823237
C	0.711051	2.917192	2.082698
C	1.071779	-4.332334	0.014345
C	-1.699295	-3.284559	-0.823237
C	-0.711051	-2.917192	2.082698
H	2.946780	-1.352726	0.895466
H	2.745005	0.406771	0.659775
H	1.829132	-0.433893	1.944980
H	2.350001	-1.763355	-2.098314
H	0.806361	-1.227657	-2.827647
H	2.036183	-0.021009	-2.351301
H	-2.946780	1.352726	0.895466
H	-2.745005	-0.406771	0.659775
H	-1.829132	0.433893	1.944980
H	-2.350001	1.763355	-2.098314
H	-0.806361	1.227657	-2.827647
H	-2.036183	0.021009	-2.351301
H	-1.383862	4.407275	-1.043051
H	-0.631891	5.303715	0.309372
H	-1.977702	4.170245	0.626182
H	1.430280	3.284064	-1.895303
H	2.128065	4.275431	-0.581982
H	2.489082	2.526718	-0.670811
H	1.157697	3.890277	2.361082
H	-0.156173	2.741170	2.744844
H	1.458155	2.128719	2.280496
H	1.383862	-4.407275	-1.043051
H	0.631891	-5.303715	0.309372
H	1.977702	-4.170245	0.626182

H	-1.430280	-3.284064	-1.895303
H	-2.128065	-4.275431	-0.581982
H	-2.489082	-2.526718	-0.670811
H	-1.157697	-3.890277	2.361082
H	0.156173	-2.741170	2.744844
H	-1.458155	-2.128719	2.280496

MP2/6311G optimized geometry, all-*eclipsed*-Si_4Me_{10}**

44
RI-MP2
Energy= -1554.06416402680065
TD B3LYP
Energy= -1557.45711058

Si	1.063538	0.522564	0.597427
Si	-1.063538	-0.522564	0.597427
Si	1.076919	2.613983	-0.482897
Si	-1.076919	-2.613983	-0.482897
C	-2.382014	0.560675	-0.240805
C	-1.605098	-0.774020	2.402353
C	2.382014	-0.560675	-0.240805
C	1.605098	0.774020	2.402353
C	2.836769	3.305929	-0.426440
C	-0.068850	3.845432	0.377817
C	0.567323	2.444585	-2.294576
C	-2.836769	-3.305929	-0.426440
C	0.068850	-3.845432	0.377817
C	-0.567323	-2.444585	-2.294576
H	-3.364740	0.078345	-0.187944
H	-2.469220	1.537724	0.246264
H	-2.156209	0.734831	-1.297867
H	-2.594750	-1.242129	2.450887
H	-0.906452	-1.415256	2.949722
H	-1.664324	0.180531	2.936703
H	3.364740	-0.078345	-0.187944
H	2.469220	-1.537724	0.246264
H	2.156209	-0.734831	-1.297867
H	2.594750	1.242129	2.450887
H	0.906452	1.415256	2.949722
H	1.664324	-0.180531	2.936703
H	3.185944	3.434922	0.603550
H	2.886477	4.285283	-0.916689
H	3.545233	2.645176	-0.937035
H	0.196867	3.966377	1.433426
H	0.000000	4.832358	-0.094392
H	-1.115652	3.529687	0.331689
H	0.649643	3.407683	-2.811764
H	1.207323	1.730861	-2.824437
H	-0.467404	2.102666	-2.395637
H	-3.185944	-3.434922	0.603550
H	-2.886477	-4.285283	-0.916689
H	-3.545233	-2.645176	-0.937035

H	-0.196867	-3.966377	1.433426
H	0.000000	-4.832358	-0.094392
H	1.115652	-3.529687	0.331689
H	-0.649643	-3.407683	-2.811764
H	-1.207323	-1.730861	-2.824437
H	0.467404	-2.102666	-2.395637

MP2/6311G optimized geometry, all-*ortho*-Si_4Me_{10}**

44
RI-MP2
Energy=-1554.06614251822157
TD B3LYP
Energy= -1557.45752553

Si	1.156236	0.229702	0.833529
Si	-1.156236	-0.229702	0.833529
Si	1.754422	1.930876	-0.679480
C	-2.145713	1.344935	0.440611
C	-1.653249	-0.803125	2.577299
Si	-1.754422	-1.930876	-0.679480
C	2.145713	-1.344935	0.440611
C	1.653249	0.803125	2.577299
C	3.640774	2.031450	-0.774293
C	1.093424	3.593802	-0.072598
C	1.087625	1.608150	-2.417166
C	-3.640774	-2.031450	-0.774293
C	-1.093424	-3.593802	-0.072598
C	-1.087625	-1.608150	-2.417166
H	-3.222703	1.154785	0.510409
H	-1.907049	2.151525	1.142832
H	-1.939715	1.712699	-0.570309
H	-2.721775	-1.042036	2.626075
H	-1.099398	-1.698255	2.879969
H	-1.453805	-0.023417	3.320479
H	3.222703	-1.154785	0.510409
H	1.907049	-2.151525	1.142832
H	1.939715	-1.712699	-0.570309
H	2.721775	1.042036	2.626075
H	1.099398	1.698255	2.879969
H	1.453805	0.023417	3.320479
H	4.083569	2.221985	0.209216
H	3.955866	2.842823	-1.440758
H	4.072945	1.101336	-1.158120
H	1.472735	3.833826	0.926348
H	1.401000	4.402622	-0.745600
H	0.000000	3.600133	-0.023795
H	1.406042	2.401322	-3.103814
H	1.450287	0.657052	-2.820573
H	-0.006709	1.577417	-2.432164
H	-4.083569	-2.221985	0.209216
H	-3.955866	-2.842823	-1.440758
H	-4.072945	-1.101336	-1.158120

H	-1.472735	-3.833826	0.926348
H	-1.401000	-4.402622	-0.745600
H	0.000000	-3.600133	-0.023795
H	-1.406042	-2.401322	-3.103814
H	-1.450287	-0.657052	-2.820573
H	0.006709	-1.577417	-2.432164

MP2/6311G optimized geometry, all-*gauche*-Si_4Me_{10}**

44
RI-MP2
Energy= -1554.06667581126726
TD B3LYP
Energy= -1557.45763764

Si	0.124487	1.169548	1.051340
Si	-0.124487	-1.169548	1.051340
Si	-0.743073	2.245772	-0.853901
C	-1.964819	-1.608076	1.227722
C	0.787641	-1.842377	2.578994
Si	0.743073	-2.245772	-0.853901
C	1.964819	1.608076	1.227722
C	-0.787641	1.842377	2.578994
C	-0.950379	4.085303	-0.466601
C	-2.429317	1.540430	-1.334170
C	0.437582	2.084620	-2.321244
C	0.950379	-4.085303	-0.466601
C	2.429317	-1.540430	-1.334170
C	-0.437582	-2.084620	-2.321244
H	-2.108878	-2.693611	1.273145
H	-2.382823	-1.181764	2.146442
H	-2.554485	-1.228561	0.387231
H	0.642169	-2.923719	2.679567
H	1.865339	-1.656602	2.518564
H	0.421705	-1.372380	3.498737
H	2.108878	2.693611	1.273145
H	2.382823	1.181764	2.146442
H	2.554485	1.228561	0.387231
H	-0.642169	2.923719	2.679567
H	-1.865339	1.656602	2.518564
H	-0.421705	1.372380	3.498737
H	-1.662119	4.245291	0.349965
H	-1.322288	4.629609	-1.342457
H	0.000000	4.543777	-0.172469
H	-3.142047	1.606227	-0.504948
H	-2.855540	2.092024	-2.180318
H	-2.357775	0.488131	-1.627894
H	0.049684	2.628629	-3.190423
H	1.422645	2.500936	-2.084397
H	0.581430	1.042648	-2.623100
H	1.662119	-4.245291	0.349965
H	1.322288	-4.629609	-1.342457
H	0.000000	-4.543777	-0.172469

H	3.142047	-1.606227	-0.504948
H	2.855540	-2.092024	-2.180318
H	2.357775	-0.488131	-1.627894
H	-0.049684	-2.628629	-3.190423
H	-1.422645	-2.500936	-2.084397
H	-0.581430	-1.042648	-2.623100

MP2/6311G optimized geometry, all-*anti*-Si_5Me_{12}**

53
RI-MP2
Energy= -1922.68379723212047
TD B3LYP
Energy= -1926.85277468

Si	0.000000	3.938779	0.474573
Si	0.000000	1.962410	-0.820203
Si	0.000000	0.000000	0.495063
Si	0.000000	-1.962410	-0.820203
Si	0.000000	-3.938779	0.474573
C	-1.544037	2.014967	-1.939291
C	1.544037	2.014967	-1.939291
C	1.543491	0.000000	1.614188
C	-1.543491	0.000000	1.614188
C	-1.544037	-2.014967	-1.939291
C	1.544037	-2.014967	-1.939291
H	-2.473332	1.959449	-1.343649
H	-1.548134	1.173252	-2.654844
H	-1.567966	2.955013	-2.521193
H	2.473332	1.959449	-1.343649
H	1.567966	2.955013	-2.521193
H	1.548134	1.173252	-2.654844
H	2.473310	0.000000	1.016802
H	1.556779	-0.894020	2.263343
H	1.556779	0.894020	2.263343
H	-2.473310	0.000000	1.016802
H	-1.556779	0.894020	2.263343
H	-1.556779	-0.894020	2.263343
H	-2.473332	-1.959449	-1.343649
H	-1.567966	-2.955013	-2.521193
H	-1.548134	-1.173252	-2.654844
H	2.473332	-1.959449	-1.343649
H	1.548134	-1.173252	-2.654844
H	1.567966	-2.955013	-2.521193
C	0.000000	-5.418678	-0.716391
C	1.542336	-4.070047	1.570281
C	-1.542336	-4.070047	1.570281
H	2.466283	-3.989261	0.969268
H	1.559854	-5.047324	2.088438
H	1.566076	-3.276654	2.338042
H	-2.466283	-3.989261	0.969268
H	-1.566076	-3.276654	2.338042
H	-1.559854	-5.047324	2.088438

H	0.000000	-6.368583	-0.148932
H	0.893885	-5.411732	-1.365982
H	-0.893885	-5.411732	-1.365982
C	0.000000	5.418678	-0.716391
C	-1.542336	4.070047	1.570281
C	1.542336	4.070047	1.570281
H	-2.466283	3.989261	0.969268
H	-1.559854	5.047324	2.088438
H	-1.566076	3.276654	2.338042
H	2.466283	3.989261	0.969268
H	1.566076	3.276654	2.338042
H	1.559854	5.047324	2.088438
H	0.000000	6.368583	-0.148932
H	-0.893885	5.411732	-1.365982
H	0.893885	5.411732	-1.365982

MP2/6311G optimized geometry, all-*transoid*-Si_5Me_{12}**

53
RI-MP2
Energy= -1922.68920291988888
TD B3LYP
Energy= -1926.85507991

C	-0.668385	-5.360195	-0.527613
Si	0.000000	-3.874669	0.433153
C	1.843133	-4.141808	0.752425
Si	-0.324718	-1.905249	-0.814002
C	-0.900720	-3.777471	2.092295
C	0.887793	-1.909818	-2.277511
C	-2.096459	-1.876933	-1.498942
Si	0.000000	0.000000	0.528147
C	1.523655	-0.224881	1.640711
Si	0.324718	1.905249	-0.814002
C	-1.523655	0.224881	1.640711
C	2.096459	1.876933	-1.498942
C	-0.887793	1.909818	-2.277511
Si	0.000000	3.874669	0.433153
C	0.900720	3.777471	2.092295 -
C	0.668385	5.360195	-0.527613 -
C	-1.843133	4.141808	0.752425 -
H	0.795491	4.716437	2.648424
H	1.971977	3.591040	1.960100
H	0.498822	2.975904	2.721208
H	-1.971977	-3.591040	1.960100
H	-0.498822	-2.975904	2.721208
H	-0.795491	-4.716437	2.648424
H	2.279459	-3.312742	1.318646
H	2.400428	-4.232653	-0.185998
H	2.010275	-5.060929	1.326069
H	-2.400428	4.232653	-0.185998
H	-2.010275	5.060929	1.326069
H	-2.279459	3.312742	1.318646
H	0.182317	5.459092	-1.504192
H	1.746024	5.272231	-0.701105
H	0.496028	6.292469	0.022844
H	-1.746024	-5.272231	-0.701105
H	-0.496028	-6.292469	0.022844
H	-0.182317	-5.459092	-1.504192
H	-2.419566	0.453837	1.053716
H	-1.373185	1.044374	2.352602
H	-1.729637	-0.681777	2.220170

H	1.729637	0.681777	2.220170
H	2.419566	-0.453837	1.053716
H	1.373185	-1.044374	2.352602
H	2.279778	2.739763	-2.149050
H	2.283227	0.972019	-2.087029
H	2.836177	1.906735	-0.691794
H	-2.283227	-0.972019	-2.087029
H	-2.836177	-1.906735	-0.691794
H	-2.279778	-2.739763	-2.149050
H	0.716634	-1.053690	-2.939240
H	0.774659	-2.818356	-2.880324
H	1.928313	-1.865900	-1.938370
H	-0.774659	2.818356	-2.880324
H	-1.928313	1.865900	-1.938370
H	-0.716634	1.053690	-2.939240

MP2/6311G optimized geometry, all-*deviant*-Si_5Me_{12}**

53
RI-MP2
Energy= -1922.68451613613001
TD B3LYP
Energy= -1926.85118986

Si	0.500370	-3.841642	0.374487
Si	-0.330864	-1.945324	-0.752530
Si	0.000000	0.000000	0.547656
Si	0.330864	1.945324	-0.752530
Si	-0.500370	3.841642	0.374487
C	0.596746	-1.866325	-2.419029
C	-2.191911	-2.129451	-1.116800
C	-1.527384	0.158327	1.680164
C	1.527384	-0.158327	1.680164
C	2.191911	2.129451	-1.116800
C	-0.596746	1.866325	-2.419029
H	1.665643	-1.627156	-2.271857
H	0.162696	-1.097646	-3.082307
H	0.535347	-2.838123	-2.943643
H	-2.776065	-2.238763	-0.185491
H	-2.378916	-3.019470	-1.745845
H	-2.574316	-1.243975	-1.658040
H	-2.452158	0.311132	1.095424
H	-1.417871	1.007980	2.378671
H	-1.654385	-0.761484	2.281580
H	2.452158	-0.311132	1.095424
H	1.417871	-1.007980	2.378671
H	1.654385	0.761484	2.281580
H	2.776065	2.238763	-0.185491
H	2.378916	3.019470	-1.745845
H	2.574316	1.243975	-1.658040
H	-1.665643	1.627156	-2.271857
H	-0.162696	1.097646	-3.082307
H	-0.535347	2.838123	-2.943643
C	0.000000	5.412191	-0.567758
C	-2.393836	3.772914	0.446970
C	0.188439	3.961028	2.138161
H	-2.827249	3.729314	-0.568716
H	-2.791712	4.676180	0.946746
H	-2.745249	2.889094	1.007516
H	1.292343	4.016764	2.129423
H	-0.102650	3.085575	2.746328
H	-0.192611	4.868046	2.644138

H	-0.402846	6.311257	-0.064194
H	-0.390012	5.399446	-1.601685
H	1.099022	5.514982	-0.619264
C	0.000000	-5.412191	-0.567758
C	2.393836	-3.772914	0.446970
C	-0.188439	-3.961028	2.138161
H	2.827249	-3.729314	-0.568716
H	2.791712	-4.676180	0.946746
H	2.745249	-2.889094	1.007516
H	-1.292343	-4.016764	2.129423
H	0.102650	-3.085575	2.746328
H	0.192611	-4.868046	2.644138
H	0.402846	-6.311257	-0.064194
H	0.390012	-5.399446	-1.601685
H	-1.099022	-5.514982	-0.619264

MP2/6311G optimized geometry, all-*eclipsed*-Si_5Me_{12}:**

53
RI-MP2
Energy= -1922.67986559886140
TD B3LYP
Energy= -1926.84824418

Si	0.000000	3.867812	0.005810
Si	0.983709	1.768642	-0.431975
Si	0.000000	0.000000	0.818658
Si	-0.983709	-1.768642	-0.431975
Si	0.000000	-3.867812	0.005810
C	0.948635	1.508311	-2.320135
C	2.823984	1.868225	0.066915
C	1.369722	-0.663407	1.970988
C	-1.369722	0.663407	1.970988
C	-2.823984	-1.868225	0.066915
C	-0.948635	-1.508311	-2.320135
H	-0.081441	1.482124	-2.716174
H	1.446545	0.564016	-2.604637
H	1.486221	2.338066	-2.815683
H	2.943206	2.069713	1.146404
H	3.329191	2.678807	-0.490682
H	3.348591	0.921792	-0.160470
H	2.223882	-1.070242	1.401831
H	0.978966	-1.463644	2.625066
H	1.750047	0.148557	2.618174
H	-2.223882	1.070242	1.401831
H	-0.978966	1.463644	2.625066
H	-1.750047	-0.148557	2.618174
H	-2.943206	-2.069713	1.146404
H	-3.329191	-2.678807	-0.490682
H	-3.348591	-0.921792	-0.160470
H	0.081441	-1.482124	-2.716174
H	-1.446545	-0.564016	-2.604637
H	-1.486221	-2.338066	-2.815683
C	-0.230147	-4.392489	1.813664
C	-0.857008	-5.160850	-1.089873
C	1.848387	-3.873037	-0.418348
H	-1.940717	-5.210193	-0.879039
H	-0.429751	-6.165013	-0.907245
H	-0.728291	-4.927287	-2.162163
H	2.414629	-3.178296	0.226741
H	2.014783	-3.577156	-1.470222
H	2.270715	-4.886282	-0.281197

H	0.174506	-5.410249	1.969422
H	-1.300485	-4.408098	2.088398
H	0.291540	-3.710504	2.507913
C	0.230147	4.392489	1.813664
C	0.857008	5.160850	-1.089873
C	-1.848387	3.873037	-0.418348
H	1.940717	5.210193	-0.879039
H	0.429751	6.165013	-0.907245
H	0.728291	4.927287	-2.162163
H	-2.414629	3.178296	0.226741
H	-2.014783	3.577156	-1.470222
H	-2.270715	4.886282	-0.281197
H	-0.174506	5.410249	1.969422
H	1.300485	4.408098	2.088398
H	-0.291540	3.710504	2.507913

MP2/6311G optimized geometry, all-*ortho*-Si_5Me_{12}**

53
RI-MP2
Energy= -1922.68754000740864
TD B3LYP
Energy= -1926.85323621

C	-2.056309	4.119952	-1.792535
Si	-2.175361	2.722610	-0.523297
C	-3.247353	1.347722	-1.251352
Si	0.000000	1.985231	-0.004089
C	-3.017719	3.392133	1.029998
C	1.002451	1.806993	-1.607244
C	0.832585	3.338082	1.042363
Si	0.000000	0.000000	1.269066
C	-1.526477	-0.013678	2.403497
Si	0.000000	-1.985231	-0.004089
C	1.526477	0.013678	2.403497
C	-0.832585	-3.338082	1.042363
C	-1.002451	-1.806993	-1.607244
Si	2.175361	-2.722610	-0.523297
C	3.017719	-3.392133	1.029998
C	2.056309	-4.119952	-1.792535
C	3.247353	-1.347722	-1.251352
H	4.015865	-3.779036	0.793905
H	2.442597	-4.211682	1.473772
H	3.134190	-2.615976	1.792851
H	-2.442597	4.211682	1.473772
H	-3.134190	2.615976	1.792851
H	-4.015865	3.779036	0.793905
H	-4.236796	1.734390	-1.522532
H	-2.799869	0.920367	-2.154562
H	-3.396894	0.531955	-0.536165
H	2.799869	-0.920367	-2.154562
H	3.396894	-0.531955	-0.536165
H	4.236796	-1.734390	-1.522532
H	1.615095	-3.771036	-2.732071
H	1.440129	-4.947065	-1.423735
H	3.048735	-4.524946	-2.022367
H	-1.440129	4.947065	-1.423735
H	-3.048735	4.524946	-2.022367
H	-1.615095	3.771036	-2.732071
H	2.459657	0.066822	1.832509
H	1.566761	-0.888170	3.025018
H	1.501527	0.878398	3.076108

H	-1.501527	-0.878398	3.076108
H	-2.459657	-0.066822	1.832509
H	-1.566761	0.888170	3.025018
H	-0.823747	-4.302664	0.521863
H	-1.877452	-3.085394	1.253543
H	-0.324168	-3.475320	2.002747
H	1.877452	3.085394	1.253543
H	0.324168	3.475320	2.002747
H	0.823747	4.302664	0.521863
H	0.554024	1.077475	-2.289502
H	1.052546	2.766393	-2.134600
H	2.029118	1.485180	-1.405195
H	-1.052546	-2.766393	-2.134600
H	-2.029118	-1.485180	-1.405195
H	-0.554024	-1.077475	-2.289502

MP2/6311G optimized geometry, all-*gauche*-Si_5Me_{12}**

53
RI-MP2
Energy= -1922.68856113997845
TD B3LYP
Energy= -1926.85331605

C	-4.107454	-2.034005	-1.382060
Si	-2.261829	-1.774007	-1.061424
C	-1.427471	-1.392420	-2.713088
Si	-2.014244	0.009968	0.457271
C	-1.541160	-3.375573	-0.364072
C	-2.238588	1.659483	-0.458945
C	-3.411289	-0.124031	1.742333
Si	0.000000	0.000000	1.673978
C	0.000000	-1.531976	2.800653
Si	2.014244	-0.009968	0.457271
C	0.000000	1.531976	2.800653
C	3.411289	0.124031	1.742333
C	2.238588	-1.659483	-0.458945
Si	2.261829	1.774007	-1.061424
C	1.541160	3.375573	-0.364072
C	4.107454	2.034005	-1.382060
C	1.427471	1.392420	-2.713088
H	1.729994	4.214345	-1.044387
H	1.985509	3.629668	0.604318
H	0.457939	3.299831	-0.224566
H	-1.985509	-3.629668	0.604318
H	-0.457939	-3.299831	-0.224566
H	-1.729994	-4.214345	-1.044387
H	-1.567934	-2.222345	-3.415585
H	-1.852309	-0.494418	-3.174548
H	-0.351048	-1.229413	-2.604800
H	1.852309	0.494418	-3.174548
H	0.351048	1.229413	-2.604800
H	1.567934	2.222345	-3.415585
H	4.579010	1.126979	-1.775766
H	4.638239	2.312199	-0.465663
H	4.267709	2.833762	-2.114477
H	-4.638239	-2.312199	-0.465663
H	-4.267709	-2.833762	-2.114477
H	-4.579010	-1.126979	-1.775766
H	0.007924	2.462562	2.224668
H	0.880155	1.537042	3.453633
H	-0.887245	1.544496	3.443855

H	0.887245	-1.544496	3.443855
H	-0.007924	-2.462562	2.224668
H	-0.880155	-1.537042	3.453633
H	4.393857	0.056416	1.262123
H	3.348632	-0.680983	2.483083
H	3.371637	1.075554	2.283325
H	-3.348632	0.680983	2.483083
H	-3.371637	-1.075554	2.283325
H	-4.393857	-0.056416	1.262123
H	-1.482157	1.803633	-1.236378
H	-3.221683	1.706530	-0.941679
H	-2.171898	2.505751	0.234215
H	3.221683	-1.706530	-0.941679
H	2.171898	-2.505751	0.234215
H	1.482157	-1.803633	-1.236378

MP2/6311G optimized geometry, all-*anti*-Si_6Me_{14}**

62
RI-MP2
Energy= -2291.30750989035323
TD B3LYP
Energy= -2296.25178749

Si	0.655461	2.939977	0.000000
C	1.767785	2.994840	1.540037
C	1.767785	2.994840	-1.540037
Si	-0.640957	4.911050	0.000000
Si	-0.658767	0.979710	0.000000
H	1.183820	2.903278	-2.462054
H	2.319557	3.940438	-1.589769
H	2.504499	2.185090	-1.532427
H	1.183820	2.903278	2.462054
H	2.504499	2.185090	1.532427
H	2.319557	3.940438	1.589769
C	-1.733208	5.034833	1.536938
C	-1.733208	5.034833	-1.536938
C	0.546281	6.384754	0.000000
H	-1.147796	4.930316	-2.456576
H	-2.509430	4.263324	-1.548296
H	-2.235246	6.008796	-1.573999
H	-1.147796	4.930316	2.456576
H	-2.235246	6.008796	1.573999
H	-2.509430	4.263324	1.548296
C	-1.767785	0.993467	-1.541510
C	-1.767785	0.993467	1.541510
Si	0.658767	-0.979710	0.000000
H	-1.174698	0.967695	2.461978
H	-2.389127	1.894572	1.573986
H	-2.438654	0.128439	1.555904
H	-1.174698	0.967695	-2.461978
H	-2.438654	0.128439	-1.555904
H	-2.389127	1.894572	-1.573986
Si	-0.655461	-2.939977	0.000000
C	-1.767785	-2.994840	-1.540037
C	-1.767785	-2.994840	1.540037
Si	0.640957	-4.911050	0.000000
H	-1.183820	-2.903278	2.462054
H	-2.504499	-2.185090	1.532427
H	-2.319557	-3.940438	1.589769
H	-1.183820	-2.903278	-2.462054
H	-2.319557	-3.940438	-1.589769

H	-2.504499	-2.185090	-1.532427
C	1.767785	-0.993467	-1.541510
C	1.767785	-0.993467	1.541510
H	1.174698	-0.967695	2.461978
H	2.389127	-1.894572	1.573986
H	2.438654	-0.128439	1.555904
H	1.174698	-0.967695	-2.461978
H	2.438654	-0.128439	-1.555904
H	2.389127	-1.894572	-1.573986
C	1.733208	-5.034833	1.536938
C	1.733208	-5.034833	-1.536938
C	-0.546281	-6.384754	0.000000
H	1.147796	-4.930316	-2.456576
H	2.509430	-4.263324	-1.548296
H	2.235246	-6.008796	-1.573999
H	1.147796	-4.930316	2.456576
H	2.235246	-6.008796	1.573999
H	2.509430	-4.263324	1.548296
H	1.192799	6.381622	0.883927
H	-0.008056	7.330645	0.000000
H	1.192799	6.381622	-0.883927
H	-1.192799	-6.381622	-0.883927
H	-1.192799	-6.381622	0.883927
H	0.008056	-7.330645	0.000000

MP2/6311G optimized geometry, all-*transoid*-Si_6Me_{14}**

62
RI-MP2
Energy= -2291.31161579193122
TD B3LYP
Energy= -2296.25229738

Si	-0.017485	1.176270	-0.023799
Si	0.017485	-1.176270	-0.023799
C	-0.676265	-1.797406	1.632061
C	-1.072495	-1.850357	-1.426235
Si	2.211959	-1.962800	-0.347825
C	1.072495	1.850357	-1.426235
Si	-2.211959	1.962800	-0.347825
C	0.676265	1.797406	1.632061
Si	2.396348	-4.218264	0.298639
C	2.652286	-1.797053	-2.188442
C	3.454594	-0.939285	0.662296
C	-3.454594	0.939285	0.662296
Si	-2.396348	4.218264	0.298639
C	-2.652286	1.797053	-2.188442
H	-0.760046	-2.890116	1.639438
H	-1.674499	-1.388447	1.822355
H	-0.033273	-1.507220	2.469998
H	1.674499	1.388447	1.822355
H	0.033273	1.507220	2.469998
H	0.760046	2.890116	1.639438
H	0.765200	1.451236	-2.398869
H	2.123769	1.582014	-1.273101
H	1.015446	2.943038	-1.483653
H	-1.015446	-2.943038	-1.483653
H	-0.765200	-1.451236	-2.398869
H	-2.123769	-1.582014	-1.273101
H	-3.214836	0.954085	1.730910
H	-3.465890	-0.106936	0.337529
H	-4.472278	1.329893	0.546479
H	4.472278	-1.329893	0.546479
H	3.214836	-0.954085	1.730910
H	3.465890	0.106936	0.337529
H	-2.576514	0.757824	-2.525911
H	-1.983994	2.398672	-2.813728
H	-3.677426	2.134404	-2.378363
H	3.677426	-2.134404	-2.378363
H	2.576514	-0.757824	-2.525911
H	1.983994	-2.398672	-2.813728

C	2.387547	-4.354013	2.183285
C	0.961704	-5.234949	-0.395451
C	4.017246	-4.943395	-0.352086
C	-0.961704	5.234949	-0.395451
C	-4.017246	4.943395	-0.352086
C	-2.387547	4.354013	2.183285
H	-3.222402	3.800311	2.625915
H	-2.480240	5.399617	2.499391
H	-1.461745	3.957912	2.612641
H	2.480240	-5.399617	2.499391
H	1.461745	-3.957912	2.612641
H	3.222402	-3.800311	2.625915
H	-4.884168	4.384402	0.016301
H	-4.052177	4.925919	-1.446443
H	-4.136372	5.985423	-0.032948
H	4.052177	-4.925919	-1.446443
H	4.136372	-5.985423	-0.032948
H	4.884168	-4.384402	0.016301
H	0.000000	4.900623	0.008183
H	-1.075488	6.294999	-0.139783
H	-0.907101	5.163272	-1.487111
H	0.907101	-5.163272	-1.487111
H	0.000000	-4.900623	0.008183
H	1.075488	-6.294999	-0.139783

MP2/6311G optimized geometry, all-*deviant*-Si_6Me_{14}**

62
RI-MP2
Energy= -2291.30502123915358
TD B3LYP
Energy= -2296.24654113

Si	0.000000	1.181329	-0.022392
Si	0.000000	-1.181329	-0.022392
C	-0.569161	-1.728892	1.713095
C	-1.225691	-1.911776	-1.289476
Si	2.103880	-2.086851	-0.605851
C	1.225691	1.911776	-1.289476
Si	-2.103880	2.086851	-0.605851
C	0.569161	1.728892	1.713095
Si	2.434007	-4.150168	0.484619
C	2.169744	-2.289305	-2.498884
C	3.563143	-0.976022	-0.075624
C	-3.563143	0.976022	-0.075624
Si	-2.434007	4.150168	0.484619
C	-2.169744	2.289305	-2.498884
H	-0.662146	-2.828849	1.770859
H	-1.558944	-1.292270	1.945069
H	0.138286	-1.402262	2.496111
H	1.558944	1.292270	1.945069
H	-0.138286	1.402262	2.496111
H	0.662146	2.828849	1.770859
H	1.048181	1.506009	-2.301943
H	2.269579	1.688364	-1.007713
H	1.116312	3.011360	-1.340789
H	-1.116312	-3.011360	-1.340789
H	-1.048181	-1.506009	-2.301943
H	-2.269579	-1.688364	-1.007713
H	-3.502494	0.718915	0.997525
H	-3.581996	0.034343	-0.651756
H	-4.525098	1.494572	-0.246588
H	4.525098	-1.494572	-0.246588
H	3.502494	-0.718915	0.997525
H	3.581996	-0.034343	-0.651756
H	-2.034047	1.313717	-3.001925
H	-1.379869	2.972113	-2.859673
H	-3.147739	2.699880	-2.811574
H	3.147739	-2.699880	-2.811574
H	2.034047	-1.313717	-3.001925
H	1.379869	-2.972113	-2.859673

C	2.661452	-3.862225	2.345011
C	0.973164	-5.329138	0.209824
C	4.004921	-4.981914	-0.182951
C	-0.973164	5.329138	0.209824
C	-4.004921	4.981914	-0.182951
C	-2.661452	3.862225	2.345011
H	-3.518665	3.192447	2.539922
H	-2.856480	4.821131	2.861186
H	-1.762246	3.407592	2.796413
H	2.856480	-4.821131	2.861186
H	1.762246	-3.407592	2.796413
H	3.518665	-3.192447	2.539922
H	-4.889668	4.334020	-0.046097
H	-3.910965	5.207210	-1.260722
H	-4.195731	5.933490	0.348373
H	3.910965	-5.207210	-1.260722
H	4.195731	-5.933490	0.348373
H	4.889668	-4.334020	-0.046097
H	-0.036240	4.914502	0.623719
H	-1.160268	6.302331	0.701583
H	-0.813637	5.519493	-0.867264
H	0.813637	-5.519493	-0.867264
H	0.036240	-4.914502	0.623719
H	1.160268	-6.302331	0.701583

MP2/6311G optimized geometry, all-*eclipsed*-Si_6Me_{14}**

62
RI-MP2
Energy= -2291.29759047917560
TD B3LYP
Energy= -2296.24121893

Si	0.113550	-4.765708	0.563446
Si	0.020252	-2.908827	-0.889717
Si	-0.751884	-0.925762	0.178128
Si	0.751884	0.925762	0.178128
Si	-0.020252	2.908827	-0.889717
Si	-0.113550	4.765708	0.563446
C	1.732113	-2.760518	-1.715575
C	-1.215595	-3.321065	-2.286085
C	-2.441520	-0.524714	-0.608760
C	-1.130421	-1.272040	2.017992
C	1.130421	1.272040	2.017992
C	2.441520	0.524714	-0.608760
C	1.215595	3.321065	-2.286085
C	-1.732113	2.760518	-1.715575
H	2.534676	-2.578856	-0.979858
H	1.754489	-1.938670	-2.453379
H	1.962556	-3.701917	-2.248291
H	-2.235260	-3.484357	-1.894264
H	-0.901125	-4.239232	-2.816443
H	-1.264728	-2.501941	-3.027260
H	-2.362308	-0.308942	-1.687976
H	-2.906911	0.348245	-0.117065
H	-3.120570	-1.388368	-0.482528
H	-0.227141	-1.567375	2.579327
H	-1.874544	-2.083610	2.111846
H	-1.550162	-0.370250	2.500975
H	0.227141	1.567375	2.579327
H	1.874544	2.083610	2.111846
H	1.550162	0.370250	2.500975
H	2.362308	0.308942	-1.687976
H	2.906911	-0.348245	-0.117065
H	3.120570	1.388368	-0.482528
H	2.235260	3.484357	-1.894264
H	0.901125	4.239232	-2.816443
H	1.264728	2.501941	-3.027260
H	-2.534676	2.578856	-0.979858
H	-1.754489	1.938670	-2.453379
H	-1.962556	3.701917	-2.248291

C	-0.751884	6.253490	-0.429789
C	-1.312474	4.467390	2.002343
C	1.594921	5.216768	1.251868
H	-2.320732	4.208574	1.630684
H	-1.403983	5.380293	2.620447
H	-0.967158	3.647241	2.656126
H	2.315016	5.402073	0.434249
H	2.003492	4.416070	1.893029
H	1.528743	6.138431	1.860142
H	-0.794162	7.154635	0.210852
H	-1.768165	6.068138	-0.821857
H	-0.091074	6.477696	-1.286720
C	0.751884	-6.253490	-0.429789
C	1.312474	-4.467390	2.002343
C	-1.594921	-5.216768	1.251868
H	2.320732	-4.208574	1.630684
H	1.403983	-5.380293	2.620447
H	0.967158	-3.647241	2.656126
H	-2.315016	-5.402073	0.434249
H	-2.003492	-4.416070	1.893029
H	-1.528743	-6.138431	1.860142
H	0.794162	-7.154635	0.210852
H	1.768165	-6.068138	-0.821857
H	0.091074	-6.477696	-1.286720

MP2/6311G optimized geometry, all-*ortho*-Si_6Me_{14}**

62
RI-MP2
Energy=-2291.30879658908725
TD B3LYP
Energy=-2296.24919951

Si	0.975345	-0.664203	-0.742732
Si	-0.975345	0.664203	-0.742732
C	-1.181788	1.382231	-2.492205
C	-2.514555	-0.397170	-0.404302
Si	-0.946811	2.434630	0.815995
C	2.514555	0.397170	-0.404302
Si	0.946811	-2.434630	0.815995
C	1.181788	-1.382231	-2.492205
Si	0.000000	4.409932	-0.050802
C	-2.754656	2.828851	1.259021
C	-0.064931	1.956090	2.428406
C	0.064931	-1.956090	2.428406
Si	0.000000	-4.409932	-0.050802
C	2.754656	-2.828851	1.259021
H	-2.068942	2.022876	-2.554558
H	-1.300448	0.580116	-3.229368
H	-0.316022	1.981956	-2.793300
H	1.300448	-0.580116	-3.229368
H	0.316022	-1.981956	-2.793300
H	2.068942	-2.022876	-2.554558
H	2.506385	0.820073	0.605693
H	2.589656	1.228831	-1.112385
H	3.423568	-0.207012	-0.502073
H	-3.423568	0.207012	-0.502073
H	-2.506385	-0.820073	0.605693
H	-2.589656	-1.228831	-1.112385
H	-0.991900	-1.721339	2.264923
H	0.534039	-1.081154	2.890213
H	0.114145	-2.778568	3.151011
H	-0.114145	2.778568	3.151011
H	0.991900	1.721339	2.264923
H	-0.534039	1.081154	2.890213
H	3.236326	-1.972636	1.743869
H	3.343001	-3.080656	0.370157
H	2.816763	-3.678380	1.948928
H	-2.816763	3.678380	1.948928
H	-3.236326	1.972636	1.743869
H	-3.343001	3.080656	0.370157

C	1.672944	4.126243	-0.880900
C	-1.177752	5.179117	-1.312647
C	0.241818	5.634603	1.370393
C	1.177752	-5.179117	-1.312647
C	-0.241818	-5.634603	1.370393
C	-1.672944	-4.126243	-0.880900
H	-2.395776	-3.672825	-0.195117
H	-2.094639	-5.077597	-1.226185
H	-1.583919	-3.469658	-1.752764
H	2.094639	5.077597	-1.226185
H	1.583919	3.469658	-1.752764
H	2.395776	3.672825	-0.195117
H	-0.957750	-5.256389	2.107656
H	0.699193	-5.834679	1.894118
H	-0.623023	-6.593172	0.999430
H	-0.699193	5.834679	1.894118
H	0.623023	6.593172	0.999430
H	0.957750	5.256389	2.107656
H	1.336698	-4.519034	-2.171195
H	0.775768	-6.126112	-1.691298
H	2.156447	-5.389933	-0.868808
H	-2.156447	5.389933	-0.868808
H	-1.336698	4.519034	-2.171195
H	-0.775768	6.126112	-1.691298

MP2/6311G optimized geometry, all-*gauche*-Si_6Me_{14}**

62
RI-MP2
Energy= -2291.31023030879942
TD B3LYP
Energy= -2296.24853945

Si	-0.285286	-1.142804	1.414622
Si	0.285286	1.142804	1.414622
C	-0.477537	1.871367	2.998154
C	2.171607	1.320582	1.579277
Si	-0.413000	2.495320	-0.381527
C	-2.171607	-1.320582	1.579277
Si	0.413000	-2.495320	-0.381527
C	0.477537	-1.871367	2.998154
Si	-2.716924	2.403193	-0.858344
C	0.000000	4.283333	0.122807
C	0.571836	2.111592	-1.959470
C	-0.571836	-2.111592	-1.959470
Si	2.716924	-2.403193	-0.858344
C	0.000000	-4.283333	0.122807
H	-0.189605	2.921632	3.121064
H	-0.132641	1.329292	3.885932
H	-1.571111	1.826317	2.983603
H	0.132641	-1.329292	3.885932
H	1.571111	-1.826317	2.983603
H	0.189605	-2.921632	3.121064
H	-2.700549	-0.956749	0.693203
H	-2.543941	-0.761578	2.445554
H	-2.449247	-2.371414	1.721923
H	2.449247	2.371414	1.721923
H	2.700549	0.956749	0.693203
H	2.543941	0.761578	2.445554
H	-0.424086	-1.081853	-2.298592
H	-1.645467	-2.257245	-1.796605
H	-0.270425	-2.777246	-2.776702
H	0.270425	2.777246	-2.776702
H	0.424086	1.081853	-2.298592
H	1.645467	2.257245	-1.796605
H	-1.061123	-4.391414	0.374189
H	0.581164	-4.602362	0.994531
H	0.218697	-4.979786	-0.694441
H	-0.218697	4.979786	-0.694441
H	1.061123	4.391414	0.374189
H	-0.581164	4.602362	0.994531

C	-3.134407	0.910556	-1.938216
C	-3.746740	2.336129	0.724363
C	-3.186614	3.967420	-1.812236
C	3.746740	-2.336129	0.724363
C	3.186614	-3.967420	-1.812236
C	3.134407	-0.910556	-1.938216
H	2.606047	-0.956790	-2.896603
H	4.208787	-0.878667	-2.154156
H	2.863207	0.035089	-1.459917
H	-4.208787	0.878667	-2.154156
H	-2.863207	-0.035089	-1.459917
H	-2.606047	0.956790	-2.896603
H	2.602471	-4.068096	-2.733471
H	3.018260	-4.868190	-1.212908
H	4.245952	-3.949349	-2.093779
H	-3.018260	4.868190	-1.212908
H	-4.245952	3.949349	-2.093779
H	-2.602471	4.068096	-2.733471
H	3.562258	-1.414773	1.285546
H	4.817506	-2.374310	0.491856
H	3.522663	-3.180550	1.385177
H	-3.522663	3.180550	1.385177
H	-3.562258	1.414773	1.285546
H	-4.817506	2.374310	0.491856

MP2/6311G optimized geometry, all-*anti*-Si7Me$_{16}$**

71
RI-MP2
Energy= -2659.92694152903687
TD B3LYP
Energy= -2665.64691553

Si	0.000000	5.893039	-0.519541
Si	0.000000	3.921910	0.776263
Si	0.000000	1.962041	-0.537932
Si	0.000000	0.000000	0.779856
Si	0.000000	-1.962041	-0.537932
Si	0.000000	-3.921910	0.776263
Si	0.000000	-5.893039	-0.519541
C	-1.537000	6.017147	-1.611529
C	0.000000	7.366921	0.667606
C	1.537000	6.017147	-1.611529
C	1.540000	3.976799	1.889269
C	-1.540000	3.976799	1.889269
C	1.542000	1.975151	-1.646930
C	-1.542000	1.975151	-1.646930
C	1.542000	0.000000	1.888838
C	-1.542000	0.000000	1.888838
C	1.542000	-1.975151	-1.646930
C	-1.542000	-1.975151	-1.646930
C	1.540000	-3.976799	1.889269
C	-1.540000	-3.976799	1.889269
C	1.537000	-6.017147	-1.611529
C	0.000000	-7.366921	0.667606
C	-1.537000	-6.017147	-1.611529
H	-2.462000	1.950092	-1.053933
H	2.462000	1.950092	-1.053933
H	2.457000	5.912089	-1.026539
H	-1.574000	2.877212	-2.267841
H	1.556000	1.110217	-2.318016
H	1.574000	2.877212	-2.267841
H	-1.556000	1.110217	-2.318016
H	1.574000	6.991197	-2.113432
H	-0.884000	7.363856	1.314605
H	0.884000	7.363856	1.314605
H	1.548000	5.245224	-2.387605
H	0.000000	8.312976	0.113700
H	-1.548000	5.245224	-2.387605
H	-2.457000	5.912089	-1.026539
H	-1.574000	6.991197	-2.113432

H	1.590000	4.921744	2.441363
H	-2.462000	3.884857	1.305260
H	-1.532000	3.166726	2.625188
H	-1.590000	4.921744	2.441363
H	2.462000	3.884857	1.305260
H	1.532000	3.166726	2.625188
H	2.462000	0.000000	1.295871
H	-2.462000	0.000000	1.295871
H	-1.556000	-0.847736	2.560968
H	-1.556000	0.847736	2.560968
H	1.556000	0.847736	2.560968
H	1.556000	-0.847736	2.560968
H	2.462000	-1.950092	-1.053933
H	-2.462000	-1.950092	-1.053933
H	-2.457000	-5.912089	-1.026539
H	1.574000	-2.877212	-2.267841
H	-1.556000	-1.110217	-2.318016
H	-1.574000	-2.877212	-2.267841
H	1.556000	-1.110217	-2.318016
H	-1.574000	-6.991197	-2.113432
H	0.884000	-7.363856	1.314605
H	-0.884000	-7.363856	1.314605
H	-1.548000	-5.245224	-2.387605
H	0.000000	-8.312976	0.113700
H	1.548000	-5.245224	-2.387605
H	2.457000	-5.912089	-1.026539
H	1.574000	-6.991197	-2.113432
H	-1.590000	-4.921744	2.441363
H	2.462000	-3.884857	1.305260
H	1.532000	-3.166726	2.625188
H	1.590000	-4.921744	2.441363
H	-2.462000	-3.884857	1.305260
H	-1.532000	-3.166726	2.625188

MP2/6311G optimized geometry, all-*transoid*-Si_7Me_{16}**

71
RI-MP2
Energy= -2659.93311243683638
TD B3LYP
Energy= -2665.64826119

Si	3.329406	4.752587	-0.395648
Si	1.674810	3.481135	0.692816
Si	1.115253	1.577232	-0.572643
Si	0.000000	0.000000	0.770666
Si	-1.115253	-1.577232	-0.572643
Si	-1.674810	-3.481135	0.692816
Si	-3.329406	-4.752587	-0.395648
C	5.005126	3.891045	-0.253871
C	3.458346	6.460955	0.405240
C	2.908649	4.976663	-2.224956
C	0.114439	4.540664	0.920564
C	2.322109	2.987039	2.410065
C	0.000000	2.121857	-2.011000
C	2.677929	0.771134	-1.291822
C	-1.286083	0.863998	1.869739
C	1.286083	-0.863998	1.869739
C	-2.677929	-0.771134	-1.291822
C	0.000000	-2.121857	-2.011000
C	-2.322109	-2.987039	2.410065
C	-0.114439	-4.540664	0.920564
C	-5.005126	-3.891045	-0.253871
C	-3.458346	-6.460955	0.405240
C	-2.908649	-4.976663	-2.224956
H	1.990482	-1.443531	1.306017
H	1.840935	-0.126951	2.477095
H	-0.805043	1.549378	2.576485
H	-1.990482	1.443531	1.306017
H	0.805043	-1.549378	2.576485
H	-1.840935	0.126951	2.477095
H	4.247516	7.056959	-0.067888
H	-0.679890	3.979828	1.424677
H	3.694966	6.387847	1.472199
H	-0.279835	4.881479	-0.042730
H	2.892325	4.017758	-2.753921
H	3.650825	5.613509	-2.720561
H	1.928585	5.447108	-2.359100
H	2.436032	-0.150360	-1.832437
H	3.395521	0.515683	-0.504680

H	3.180870	1.444445	-1.995235
H	-0.955345	2.516931	-1.649094
H	-0.218794	1.282649	-2.680697
H	0.477399	2.906005	-2.609084
H	5.300987	3.766321	0.793220
H	2.520529	7.018435	0.311111
H	3.193062	2.326815	2.338072
H	1.553882	2.463611	2.989745
H	2.623272	3.869792	2.986015
H	0.328665	5.429513	1.524586
H	5.787762	4.476241	-0.750689
H	4.989377	2.898278	-0.714867
H	-4.247516	-7.056959	-0.067888
H	0.679890	-3.979828	1.424677
H	-3.694966	-6.387847	1.472199
H	0.279835	-4.881479	-0.042730
H	-2.892325	-4.017758	-2.753921
H	-3.650825	-5.613509	-2.720561
H	-1.928585	-5.447108	-2.359100
H	-2.436032	0.150360	-1.832437
H	-3.395521	-0.515683	-0.504680
H	-3.180870	-1.444445	-1.995235
H	0.955345	-2.516931	-1.649094
H	0.218794	-1.282649	-2.680697
H	-0.477399	-2.906005	-2.609084
H	-5.300987	-3.766321	0.793220
H	-2.520529	-7.018435	0.311111
H	-3.193062	-2.326815	2.338072
H	-1.553882	-2.463611	2.989745
H	-2.623272	-3.869792	2.986015
H	-0.328665	-5.429513	1.524586
H	-5.787762	-4.476241	-0.750689
H	-4.989377	-2.898278	-0.714867

MP2/6311G optimized geometry, all-*deviant*-Si_7Me_{16}**

71
RI-MP2
Energy= -2659.91885021713597
TD B3LYP
Energy= -2665.63565051

Si	0.000000	5.812490	-0.181458
Si	-1.017726	3.786271	0.462012
Si	0.051986	1.962548	-0.594612
Si	0.000000	0.000000	0.718479
Si	-0.051986	-1.962548	-0.594612
Si	1.017726	-3.786271	0.462012
Si	0.000000	-5.812490	-0.181458
C	1.738461	5.922311	0.567804
C	-1.019947	7.275413	0.470301
C	0.123118	5.966045	-2.068467
C	-0.891676	3.719473	2.365741
C	-2.862697	3.760647	-0.011620
C	1.885856	2.319197	-0.975938
C	-0.853843	1.750620	-2.260725
C	1.557317	0.095245	1.819082
C	-1.557317	-0.095245	1.819082
C	0.853843	-1.750620	-2.260725
C	-1.885856	-2.319197	-0.975938
C	2.862697	-3.760647	-0.011620
C	0.891676	-3.719473	2.365741
C	-0.123118	-5.966045	-2.068467
C	1.019947	-7.275413	0.470301
C	-1.738461	-5.922311	0.567804
H	-3.000623	3.855614	-1.103525
H	0.573461	6.936042	-2.351725
H	-2.035248	7.280918	0.034058
H	-0.532681	8.234257	0.210681
H	0.748419	5.163115	-2.499003
H	-0.875934	5.907003	-2.537735
H	1.988486	3.189872	-1.649197
H	2.347714	1.447237	-1.476431
H	2.460752	2.526714	-0.055767
H	-1.121730	7.233793	1.569928
H	-3.400328	4.594771	0.476245
H	-3.336823	2.815193	0.311734
H	-0.907249	2.717593	-2.795319
H	-1.887052	1.386935	-2.114235
H	-0.325736	1.032524	-2.912222

H	2.210165	6.887697	0.304181
H	2.389824	5.111163	0.197951
H	1.699281	5.854601	1.670205
H	-1.285777	4.651817	2.811723
H	0.156988	3.603055	2.694649
H	-1.474351	2.877220	2.778227
H	-1.500023	-0.992388	2.472427
H	-2.462624	-0.047438	1.299054
H	2.462624	0.047438	1.299054
H	1.545445	-0.690651	2.594473
H	1.500023	0.992388	2.472427
H	-1.545445	0.690651	2.594473
H	3.000623	-3.855614	-1.103525
H	-0.573461	-6.936042	-2.351725
H	2.035248	-7.280918	0.034058
H	0.532681	-8.234257	0.210681
H	-0.748419	-5.163115	-2.499003
H	0.875934	-5.907003	-2.537735
H	-1.988486	-3.189872	-1.649197
H	-2.347714	-1.447237	-1.476431
H	-2.460752	-2.526714	-0.055767
H	1.121730	-7.233793	1.569928
H	3.400328	-4.594771	0.476245
H	3.336823	-2.815193	0.311734
H	0.907249	-2.717593	-2.795319
H	1.887052	-1.386935	-2.114235
H	0.325736	-1.032524	-2.912222
H	-2.210165	-6.887697	0.304181
H	-2.389824	-5.111163	0.197951
H	-1.699281	-5.854601	1.670205
H	1.285777	-4.651817	2.811723
H	-0.156988	-3.603055	2.694649
H	1.474351	-2.877220	2.778227

MP2/6311G optimized geometry, all-*eclipsed*-Si_7Me_{16}**

71
RI-MP2
Energy= -2659.90157409929043
TD B3LYP
Energy= -2665.62069465

Si	1.054527	5.643416	0.513086
Si	-0.347355	3.930874	-0.305645
Si	0.794574	1.867901	-0.636067
Si	0.000000	0.000000	0.615213
Si	-0.794574	-1.867901	-0.636067
Si	0.347355	-3.930874	-0.305645
Si	-1.054527	-5.643416	0.513086
C	1.789348	5.196596	2.203420
C	0.000000	7.208177	0.729834
C	2.458411	6.051749	-0.694648
C	-1.852206	3.836667	0.860998
C	-1.019054	4.487663	-2.004441
C	2.633446	2.047004	-0.151536
C	0.805055	1.564570	-2.518294
C	1.439605	-0.516545	1.742398
C	-1.439605	0.516545	1.742398
C	-0.805055	-1.564570	-2.518294
C	-2.633446	-2.047004	-0.151536
C	1.019054	-4.487663	-2.004441
C	1.852206	-3.836667	0.860998
C	-2.458411	-6.051749	-0.694648
C	0.000000	-7.208177	0.729834
C	-1.789348	-5.196596	2.203420
H	3.044428	6.911988	-0.319935
H	-0.813088	7.046256	1.460293
H	2.059213	6.321892	-1.689152
H	2.462777	4.324060	2.136372
H	3.149953	5.200606	-0.822956
H	2.372307	6.046860	2.604706
H	-1.562328	3.576635	1.893829
H	-2.585374	3.086625	0.514315
H	-2.357340	4.820239	0.884417
H	-0.206402	4.627690	-2.739215
H	-1.560934	5.446747	-1.905815
H	-1.723492	3.741615	-2.416629
H	-0.211572	1.448851	-2.931353
H	1.382415	0.656131	-2.766893
H	1.284198	2.421905	-3.026567

H	2.759883	2.276686	0.920610
H	3.108305	2.856372	-0.735150
H	3.180655	1.110051	-0.364514
H	0.623912	8.045309	1.096187
H	0.992365	4.959750	2.931719
H	-0.457484	7.519895	-0.226623
H	-3.044428	-6.911988	-0.319935
H	0.813088	-7.046256	1.460293
H	-2.059213	-6.321892	-1.689152
H	-2.462777	-4.324060	2.136372
H	-3.149953	-5.200606	-0.822956
H	-2.372307	-6.046860	2.604706
H	1.562328	-3.576635	1.893829
H	2.585374	-3.086625	0.514315
H	2.357340	-4.820239	0.884417
H	0.206402	-4.627690	-2.739215
H	1.560934	-5.446747	-1.905815
H	1.723492	-3.741615	-2.416629
H	0.211572	-1.448851	-2.931353
H	-1.382415	-0.656131	-2.766893
H	-1.284198	-2.421905	-3.026567
H	-2.759883	-2.276686	0.920610
H	-3.108305	-2.856372	-0.735150
H	-3.180655	-1.110051	-0.364514
H	-0.623912	-8.045309	1.096187
H	-0.992365	-4.959750	2.931719
H	0.457484	-7.519895	-0.226623
H	-1.127567	1.270694	2.487456
H	-1.682924	-0.427233	2.426982
H	-2.342907	0.769608	1.275801
H	2.342907	-0.769608	1.275801
H	1.127567	-1.270694	2.487456
H	1.682924	0.427233	2.426982

MP2/6311G optimized geometry, all-*ortho*-Si_7Me_{16}**

71
RI-MP2
Energy= -2659.92385955784721
TD B3LYP
Energy= -2665.63811419

Si	1.002262	5.105383	0.654010
Si	0.602510	3.425594	-0.948523
Si	1.475005	1.325641	-0.320985
Si	0.000000	0.000000	0.953587
Si	-1.475005	-1.325641	-0.320985
Si	-0.602510	-3.425594	-0.948523
Si	-1.002262	-5.105383	0.654010
C	0.509873	4.591068	2.403672
C	0.000000	6.638276	0.180935
C	2.835842	5.562526	0.652228
C	-1.254056	3.342752	-1.339528
C	1.490925	3.954017	-2.545857
C	2.011624	0.412638	-1.898540
C	3.047193	1.592772	0.716179
C	-1.065964	1.133763	2.049708
C	1.065964	-1.133763	2.049708
C	-2.011624	-0.412638	-1.898540
C	-3.047193	-1.592772	0.716179
C	-1.490925	-3.954017	-2.545857
C	1.254056	-3.342752	-1.339528
C	-2.835842	-5.562526	0.652228
C	0.000000	-6.638276	0.180935
C	-0.509873	-4.591068	2.403672
H	1.103849	3.741220	2.755993
H	2.577291	3.990153	-2.411178
H	3.463704	4.714015	0.941872
H	-0.545607	4.306652	2.462331
H	0.206525	7.467324	0.867821
H	-1.076323	6.439584	0.215713
H	0.670072	5.418649	3.104791
H	3.772766	2.216099	0.181051
H	3.533019	0.635866	0.937948
H	2.828946	2.081570	1.671859
H	1.164063	4.948863	-2.869846
H	1.281115	3.254340	-3.362324
H	2.771194	0.992331	-2.435112
H	1.173143	0.252577	-2.584350
H	2.442639	-0.566588	-1.666114

H	3.163240	5.896527	-0.337991
H	0.241551	6.980858	-0.831049
H	3.032848	6.378037	1.357848
H	-1.618482	4.319216	-1.678292
H	-1.845840	3.053303	-0.465036
H	-1.457906	2.618985	-2.135422
H	-0.439072	1.789309	2.665033
H	1.638999	-0.449378	2.787393
H	-1.638999	0.449378	2.787393
H	-1.731232	1.770165	1.456166
H	1.731232	-1.770165	1.456166
H	0.439072	-1.789309	2.665033
H	-1.103849	-3.741220	2.755993
H	-2.577291	-3.990153	-2.411178
H	-3.463704	-4.714015	0.941872
H	0.545607	-4.306652	2.462331
H	-0.206525	-7.467324	0.867821
H	1.076323	-6.439584	0.215713
H	-0.670072	-5.418649	3.104791
H	-3.772766	-2.216099	0.181051
H	-3.533019	-0.635866	0.937948
H	-2.828946	-2.081570	1.671859
H	-1.164063	-4.948863	-2.869846
H	-1.281115	-3.254340	-3.362324
H	-2.771194	-0.992331	-2.435112
H	-1.173143	-0.252577	-2.584350
H	-2.442639	0.566588	-1.666114
H	-3.163240	-5.896527	-0.337991
H	-0.241551	-6.980858	-0.831049
H	-3.032848	-6.378037	1.357848
H	1.618482	-4.319216	-1.678292
H	1.845840	-3.053303	-0.465036
H	1.457906	-2.618985	-2.135422

MP2/6311G optimized geometry, all-*gauche*-Si_7Me_{16}**

71
RI-MP2
Energy= -2659.89747270114731
TD B3LYP
Energy= -2665.61064340

Si	0.890813	-4.425275	-0.173670
Si	-0.705772	-2.944036	-1.068520
Si	-1.526868	-1.336041	0.442510
Si	0.000000	0.000000	1.631785
Si	1.526868	1.336041	0.442510
Si	0.705772	2.944036	-1.068520
Si	-0.890813	4.425275	-0.173670
C	0.926726	-5.978524	-1.252305
C	0.447576	-4.933161	1.591427
C	2.618501	-3.661558	-0.188079
C	0.000000	-2.127346	-2.631196
C	-2.214092	-3.975377	-1.600705
C	-2.741730	-0.216975	-0.500212
C	-2.540165	-2.264931	1.758058
C	-0.987444	1.096589	2.830837
C	0.987444	-1.096589	2.830837
C	2.540165	2.264931	1.758058
C	2.741730	0.216975	-0.500212
C	2.214092	3.975377	-1.600705
C	0.000000	2.127346	-2.631196
C	-0.447576	4.933161	1.591427
C	-0.926726	5.978524	-1.252305
C	-2.618501	3.661558	-0.188079
H	-3.005318	-3.340001	-2.014363
H	-0.036910	-6.498284	-1.238891
H	-0.555858	-5.369425	1.643637
H	2.667763	-2.738314	0.396522
H	1.159891	-5.739162	-2.295556
H	1.153316	-5.683130	1.967640
H	1.688436	-6.682481	-0.897299
H	0.476327	-4.078915	2.275015
H	-2.641427	-4.531201	-0.759350
H	-3.013608	-1.565112	2.455951
H	-1.919687	-2.951126	2.343114
H	-3.337472	-2.853940	1.290682
H	-2.253011	0.337037	-1.307371
H	-3.206811	0.511960	0.173514
H	-3.546684	-0.811693	-0.947472

H	3.352919	-4.360119	0.229752
H	-1.937057	-4.702699	-2.372084
H	0.852037	-1.477806	-2.409095
H	-0.760361	-1.518564	-3.132851
H	0.337911	-2.885946	-3.346846
H	2.934990	-3.420834	-1.208713
H	1.660109	-1.848134	2.085912
H	-1.660109	1.848134	2.085912
H	-0.318293	1.695258	3.459635
H	0.318293	-1.695258	3.459635
H	1.752058	-0.598011	3.334578
H	-1.752058	0.598011	3.334578
H	3.005318	3.340001	-2.014363
H	0.036910	6.498284	-1.238891
H	0.555858	5.369425	1.643637
H	-2.667763	2.738314	0.396522
H	-1.159891	5.739162	-2.295556
H	-1.153316	5.683130	1.967640
H	-1.688436	6.682481	-0.897299
H	-0.476327	4.078915	2.275015
H	2.641427	4.531201	-0.759350
H	3.013608	1.565112	2.455951
H	1.919687	2.951126	2.343114
H	3.337472	2.853940	1.290682
H	2.253011	-0.337037	-1.307371
H	3.206811	-0.511960	0.173514
H	3.546684	0.811693	-0.947472
H	-3.352919	4.360119	0.229752
H	1.937057	4.702699	-2.372084
H	-0.852037	1.477806	-2.409095
H	0.760361	1.518564	-3.132851
H	-0.337911	2.885946	-3.346846
H	-2.934990	3.420834	-1.208713

MP2/6311G optimized geometry, all-*anti*-Si_8Me_{18}**

80
RI-MP2
Energy= -3028.54937069128300
TD B3LYP
Energy= -3035.04457862

H	-1.174314	-2.929721	-2.462000
H	-1.174314	-2.929721	2.462000
C	-1.729472	-6.997109	-1.537000
H	-1.144546	-6.891701	2.457000
Si	-0.637559	-6.872346	0.000000
C	0.550470	-8.345517	0.000000
C	-1.729472	-6.997109	1.537000
H	-2.387666	-3.857569	-1.574000
H	-2.438901	-2.090604	1.556000
H	-2.387666	-3.857569	1.574000
H	-2.438901	-2.090604	-1.556000
H	-2.230792	-7.971460	1.574000
H	1.197468	-8.342065	-0.884000
H	1.197468	-8.342065	0.884000
H	-2.506012	-6.225652	1.548000
H	-0.002868	-9.291904	0.000000
H	-2.506012	-6.225652	-1.548000
H	-1.144546	-6.891701	-2.457000
H	-2.230792	-7.971460	-1.574000
Si	0.658306	-0.980466	0.000000
H	2.322762	-5.899278	1.590000
H	1.186037	-4.863072	-2.462000
Si	-0.658306	-2.941360	0.000000
H	2.505535	-4.144149	-1.532000
H	2.322762	-5.899278	-1.590000
H	1.186037	-4.863072	2.462000
H	2.505535	-4.144149	1.532000
C	-1.767297	-2.955135	1.542000
C	-1.767297	-2.955135	-1.542000
Si	0.657063	-4.900441	0.000000
C	1.770101	-4.954664	1.540000
C	1.770101	-4.954664	-1.540000
H	-1.174314	0.968832	2.462000
C	1.767297	-0.994251	-1.542000
H	-1.174314	0.968832	-2.462000
C	1.767297	-0.994251	1.542000
H	-2.438909	0.129727	-1.556000
H	-2.387658	1.896691	-1.574000

H	-2.387658	1.896691	1.574000
Si	-0.658306	0.980466	0.000000
H	2.438909	-0.129727	1.556000
H	-2.438909	0.129727	1.556000
H	1.174314	-0.968832	-2.462000
H	2.438909	-0.129727	-1.556000
C	-1.767297	0.994251	-1.542000
H	2.387658	-1.896691	-1.574000
H	1.174314	-0.968832	2.462000
Si	0.658306	2.941360	0.000000
C	-1.767297	0.994251	1.542000
H	2.387658	-1.896691	1.574000
H	1.174314	2.929721	-2.462000
H	1.174314	2.929721	2.462000
C	1.729472	6.997109	-1.537000
H	1.144546	6.891701	2.457000
Si	0.637559	6.872346	0.000000
C	-0.550470	8.345517	0.000000
C	1.729472	6.997109	1.537000
H	2.387666	3.857569	-1.574000
H	2.438901	2.090604	1.556000
H	2.387666	3.857569	1.574000
H	2.438901	2.090604	-1.556000
H	2.230792	7.971460	1.574000
H	-1.197468	8.342065	-0.884000
H	-1.197468	8.342065	0.884000
H	2.506012	6.225652	1.548000
H	0.002868	9.291904	0.000000
H	2.506012	6.225652	-1.548000
H	1.144546	6.891701	-2.457000
H	2.230792	7.971460	-1.574000
H	-2.322762	5.899278	1.590000
H	-1.186037	4.863072	-2.462000
H	-2.505535	4.144149	-1.532000
H	-2.322762	5.899278	-1.590000
H	-1.186037	4.863072	2.462000
H	-2.505535	4.144149	1.532000
C	1.767297	2.955135	1.542000
C	1.767297	2.955135	-1.542000
Si	-0.657063	4.900441	0.000000
C	-1.770101	4.954664	1.540000
C	-1.770101	4.954664	-1.540000

MP2/6311G optimized geometry, all-*transoid*-Si_8Me_{18}**

80
RI-MP2
Energy= -3028.55549438392836
TD B3LYP
Energy= -3035.04517381

Si	-0.691661	0.951589	-0.181318
Si	0.691661	-0.951589	-0.181318
C	1.983949	-0.767338	1.198905
C	1.600151	-1.104474	-1.842808
H	-0.897209	1.127694	-2.682497
C	-1.600151	1.104474	-1.842808
H	2.279716	-0.259515	-2.000512
C	-1.983949	0.767338	1.198905
H	-2.279716	0.259515	-2.000512
H	-2.197942	2.021694	-1.885895
H	2.197942	-2.021694	-1.885895
Si	0.591805	2.896699	0.142616
Si	-0.591805	-2.896699	0.142616
H	0.897209	-1.127694	-2.682497
H	2.704746	-1.592600	1.176907
H	2.547378	0.166050	1.092773
H	1.514930	-0.761356	2.188738
H	-2.547378	-0.166050	1.092773
H	-1.514930	0.761356	2.188738
H	-2.704746	1.592600	1.176907
C	2.192343	6.761943	0.169368
C	-0.409716	8.279612	-0.421556
H	0.000000	9.199547	0.011705
H	-1.076981	4.034698	-2.841409
C	2.169748	2.827007	-0.913090
Si	-0.636858	4.802947	-0.486624
C	1.093214	2.999945	1.972069
C	-0.049460	6.851017	2.273018
H	-1.498672	8.319150	-0.310435
H	0.377547	5.037838	-2.775388
C	-2.437026	4.675938	0.109473
Si	0.318976	6.752082	0.422379
C	-0.638745	4.927353	-2.382343
H	2.673943	5.934046	0.700608
H	2.631543	7.693793	0.544573
H	2.457094	6.676009	-0.890048
H	1.613320	2.090781	2.292759
H	0.219723	3.128952	2.620264

H	1.767113	3.845887	2.149074
H	1.935788	2.680717	-1.973093
H	2.819293	2.002557	-0.598435
H	2.747180	3.754122	-0.826288
H	-1.127744	6.876172	2.463180
H	-0.185289	8.289506	-1.493319
H	-2.493945	4.546212	1.195553
H	-2.951418	3.827563	-0.355113
H	-3.000650	5.580985	-0.145254
H	-1.220245	5.793386	-2.717951
H	0.383989	7.758695	2.708959
H	0.363009	5.993112	2.813592
C	-2.192343	-6.761943	0.169368
C	0.409716	-8.279612	-0.421556
H	0.000000	-9.199547	0.011705
H	1.076981	-4.034698	-2.841409
C	-2.169748	-2.827007	-0.913090
Si	0.636858	-4.802947	-0.486624
C	-1.093214	-2.999945	1.972069
C	0.049460	-6.851017	2.273018
H	1.498672	-8.319150	-0.310435
H	-0.377547	-5.037838	-2.775388
C	2.437026	-4.675938	0.109473
Si	-0.318976	-6.752082	0.422379
C	0.638745	-4.927353	-2.382343
H	-2.673943	-5.934046	0.700608
H	-2.631543	-7.693793	0.544573
H	-2.457094	-6.676009	-0.890048
H	-1.613320	-2.090781	2.292759
H	-0.219723	-3.128952	2.620264
H	-1.767113	-3.845887	2.149074
H	-1.935788	-2.680717	-1.973093
H	-2.819293	-2.002557	-0.598435
H	-2.747180	-3.754122	-0.826288
H	1.127744	-6.876172	2.463180
H	0.185289	-8.289506	-1.493319
H	2.493945	-4.546212	1.195553
H	2.951418	-3.827563	-0.355113
H	3.000650	-5.580985	-0.145254
H	1.220245	-5.793386	-2.717951
H	-0.383989	-7.758695	2.708959
H	-0.363009	-5.993112	2.813592

MP2/6311G optimized geometry, all-*deviant*-Si_8Me_{18}**

80
RI-MP2
Energy= -3028.54588122135783
TD B3LYP
Energy= -3035.03721543

H	1.602099	5.191121	2.324464
Si	1.229251	2.695418	-0.281982
C	1.341914	2.770130	-2.183931
C	-0.327218	3.666550	0.243071
Si	3.032519	3.804001	0.769669
C	4.691207	4.811342	-2.129374
H	2.831552	7.519076	-1.785303
H	4.646810	7.061334	1.233235
Si	3.833370	5.543186	-0.604834
C	2.432525	4.473394	2.449198
C	4.526034	2.657693	1.085778
H	5.520908	7.375821	-0.294774
H	1.683567	6.148840	-1.772897
H	1.911091	7.137286	-0.301640
H	1.331942	3.816338	-2.540633
H	0.477921	2.248892	-2.637749
H	2.263484	2.288662	-2.556999
H	5.946788	5.954876	0.702724
H	3.255533	4.989009	2.977990
H	2.077360	3.648785	3.095042
C	5.105487	6.579197	0.351002
C	2.432525	6.691849	-1.168528
Si	1.108255	0.409034	0.301249
H	-0.187014	4.747912	0.056842
H	-0.541622	3.533023	1.318918
H	-1.213128	3.337012	-0.327519
H	5.105564	5.619001	-2.761804
H	3.988722	4.221865	-2.744237
H	5.526289	4.150266	-1.834379
H	5.389897	3.241887	1.454477
H	4.837118	2.139512	0.160497
H	4.290937	1.890481	1.844170
Si	-1.108255	-0.409034	0.301249
C	1.819019	0.064673	2.036736
C	2.217913	-0.487922	-0.965835
H	-1.775783	0.461889	-1.978302
C	-2.217913	0.487922	-0.965835
H	2.369766	-1.544594	-0.684072

C	-1.819019	-0.064673	2.036736
H	-2.369766	1.544594	-0.684072
H	-3.211607	0.004580	-1.017148
H	3.211607	-0.004580	-1.017148
Si	-1.229251	-2.695418	-0.281982
H	1.775783	-0.461889	-1.978302
H	2.883131	0.358299	2.094500
H	1.752116	-1.015065	2.268710
H	1.267640	0.615264	2.819752
H	-1.752116	1.015065	2.268710
H	-1.267640	-0.615264	2.819752
H	-2.883131	-0.358299	2.094500
H	-1.602099	-5.191121	2.324464
C	-1.341914	-2.770130	-2.183931
C	0.327218	-3.666550	0.243071
Si	-3.032519	-3.804001	0.769669
C	-4.691207	-4.811342	-2.129374
H	-2.831552	-7.519076	-1.785303
H	-4.646810	-7.061334	1.233235
Si	-3.833370	-5.543186	-0.604834
C	-2.432525	-4.473394	2.449198
C	-4.526034	-2.657693	1.085778
H	-5.520908	-7.375821	-0.294774
H	-1.683567	-6.148840	-1.772897
H	-1.911091	-7.137286	-0.301640
H	-1.331942	-3.816338	-2.540633
H	-0.477921	-2.248892	-2.637749
H	-2.263484	-2.288662	-2.556999
H	-5.946788	-5.954876	0.702724
H	-3.255533	-4.989009	2.977990
H	-2.077360	-3.648785	3.095042
C	-5.105487	-6.579197	0.351002
C	-2.432525	-6.691849	-1.168528
H	0.187014	-4.747912	0.056842
H	0.541622	-3.533023	1.318918
H	1.213128	-3.337012	-0.327519
H	-5.105564	-5.619001	-2.761804
H	-3.988722	-4.221865	-2.744237
H	-5.526289	-4.150266	-1.834379
H	-5.389897	-3.241887	1.454477
H	-4.837118	-2.139512	0.160497
H	-4.290937	-1.890481	1.844170

MP2/6311G optimized geometry, all-*eclipsed*-Si_8Me_{18}**

80
RI-MP2
Energy= -3028.53250887934109
TD B3LYP
Energy= -3035.02611409

Si	-6.725580	-0.368467	-0.156206
Si	-4.689684	-1.277204	0.616916
Si	-2.828700	-0.693671	-0.748831
H	-8.171144	-0.621721	-2.183302
H	-7.916627	-0.536400	2.058821
C	-8.099308	-0.913987	1.036590
C	-4.522203	-0.788639	2.452062
C	-4.847747	-3.180036	0.580186
C	-2.239212	-2.314912	-1.560607
C	-3.396315	0.410783	-2.200137
H	-7.211851	-2.104225	-1.908423
H	-5.941192	1.912940	-0.890265
H	-6.446088	-0.667130	-2.647107
H	-7.674485	1.930555	-0.453293
H	-4.481977	0.305871	2.589241
H	-3.611857	-1.221822	2.903626
H	-5.395135	-1.172152	3.012445
H	-5.008384	-3.556987	-0.445488
H	-5.702372	-3.504927	1.202491
H	-3.935927	-3.661834	0.979151
H	-1.886305	-3.052309	-0.819499
H	-1.416338	-2.121851	-2.271954
H	-3.075458	-2.770088	-2.123145
H	-3.810261	1.373063	-1.852428
H	-4.173320	-0.103444	-2.794282
H	-2.546123	0.630318	-2.872191
H	-9.078587	-0.523795	0.700389
H	-6.430905	1.925415	0.829855
H	-8.172905	-2.015462	1.087651
C	-7.174616	-0.999900	-1.887076
C	-6.684000	1.527561	-0.169822
Si	-1.074378	0.517762	0.320955
H	-0.846145	2.227102	-1.545149
H	0.718238	-1.422751	2.643802
Si	1.074378	-0.517762	0.320955
H	-0.332495	2.908754	0.025762
H	-2.071506	2.715581	-0.339701
H	0.846145	-2.227102	-1.545149

H	-1.577462	-0.140971	2.722154
C	1.074378	-2.254341	-0.465933
C	1.498715	-0.806096	2.160819
C	-1.498715	0.806096	2.160819
C	-1.074378	2.254341	-0.465933
H	0.332495	-2.908754	0.025762
H	2.071506	-2.715581	-0.339701
H	1.577462	0.140971	2.722154
H	2.460195	-1.342679	2.254673
H	-2.460195	1.342679	2.254673
H	-0.718238	1.422751	2.643802
Si	2.828700	0.693671	-0.748831
Si	6.725580	0.368467	-0.156206
Si	4.689684	1.277204	0.616916
H	8.171144	0.621721	-2.183302
H	7.916627	0.536400	2.058821
C	8.099308	0.913987	1.036590
C	4.522203	0.788639	2.452062
C	4.847747	3.180036	0.580186
C	2.239212	2.314912	-1.560607
C	3.396315	-0.410783	-2.200137
H	7.211851	2.104225	-1.908423
H	5.941192	-1.912940	-0.890265
H	6.446088	0.667130	-2.647107
H	7.674485	-1.930555	-0.453293
H	4.481977	-0.305871	2.589241
H	3.611857	1.221822	2.903626
H	5.395135	1.172152	3.012445
H	5.008384	3.556987	-0.445488
H	5.702372	3.504927	1.202491
H	3.935927	3.661834	0.979151
H	1.886305	3.052309	-0.819499
H	1.416338	2.121851	-2.271954
H	3.075458	2.770088	-2.123145
H	3.810261	-1.373063	-1.852428
H	4.173320	0.103444	-2.794282
H	2.546123	-0.630318	-2.872191
H	9.078587	0.523795	0.700389
H	6.430905	-1.925415	0.829855
H	8.172905	2.015462	1.087651
C	7.174616	0.999900	-1.887076
C	6.684000	-1.527561	-0.169822

MP2/6311G optimized geometry, all-*ortho*-Si_8Me_{18}**

80
RI-MP2
Energy= -3028.5515471675
TD B3LYP
Energy= -3035.03919912

H	-2.262257	4.715851	-1.635343
Si	-0.443082	2.573394	1.110755
C	-2.137141	3.284889	1.603477
C	0.343554	1.889541	2.699391
Si	0.921553	4.322973	0.309755
H	1.031820	5.479069	2.547863
H	-2.026984	6.382714	1.005206
H	-0.972577	4.763079	-2.844122
Si	-0.299107	6.019436	-0.777264
C	1.764892	5.119707	1.817727
C	2.298661	3.691289	-0.835292
H	0.396463	8.028525	-2.095379
H	1.486321	6.672781	-2.413755
H	-2.001317	6.179093	-2.591597
H	-2.027554	4.106173	2.321001
H	-2.759284	2.515231	2.074054
H	-2.686807	3.670025	0.737789
Si	-0.822616	0.843026	-0.448684
H	2.382292	5.975024	1.519771
H	2.416990	4.402420	2.328077
C	-1.491615	5.352952	-2.081874
C	-1.286694	7.007342	0.495415
C	0.921553	7.186812	-1.628918
H	0.427071	2.679478	3.454325
H	1.349533	1.495421	2.521400
H	-0.258975	1.081930	3.127649
H	-0.632834	7.440135	1.259900
H	1.644135	7.602290	-0.918233
H	-1.823450	7.832983	0.013774
H	2.946533	4.518007	-1.148101
H	1.898263	3.223223	-1.740456
H	2.926823	2.952500	-0.326919
Si	0.822616	-0.843026	-0.448684
C	-0.830957	1.564381	-2.209324
C	-2.530777	0.055559	-0.167608
H	2.634431	0.359799	0.839376
C	2.530777	-0.055559	-0.167608

H	2.712337	0.753389	-0.884680
C	0.830957	-1.564381	-2.209324
H	3.325259	-0.798773	-0.302186
Si	0.443082	-2.573394	1.110755
H	-3.325259	0.798773	-0.302186
H	-2.634431	-0.359799	0.839376
H	-2.712337	-0.753389	-0.884680
H	-1.630334	2.305532	-2.322280
H	-1.001831	0.779523	-2.954809
H	0.115489	2.056770	-2.454148
H	1.001831	-0.779523	-2.954809
H	-0.115489	-2.056770	-2.454148
H	1.630334	-2.305532	-2.322280
H	2.262257	-4.715851	-1.635343
C	2.137141	-3.284889	1.603477
C	-0.343554	-1.889541	2.699391
Si	-0.921553	-4.322973	0.309755
H	-1.031820	-5.479069	2.547863
H	2.026984	-6.382714	1.005206
H	0.972577	-4.763079	-2.844122
Si	0.299107	-6.019436	-0.777264
C	-1.764892	-5.119707	1.817727
C	-2.298661	-3.691289	-0.835292
H	-0.396463	-8.028525	-2.095379
H	-1.486321	-6.672781	-2.413755
H	2.001317	-6.179093	-2.591597
H	2.027554	-4.106173	2.321001
H	2.759284	-2.515231	2.074054
H	2.686807	-3.670025	0.737789
H	-2.382292	-5.975024	1.519771
H	-2.416990	-4.402420	2.328077
C	1.491615	-5.352952	-2.081874
C	1.286694	-7.007342	0.495415
C	-0.921553	-7.186812	-1.628918
H	-0.427071	-2.679478	3.454325
H	-1.349533	-1.495421	2.521400
H	0.258975	-1.081930	3.127649
H	0.632834	-7.440135	1.259900
H	-1.644135	-7.602290	-0.918233
H	1.823450	-7.832983	0.013774
H	-2.946533	-4.518007	-1.148101
H	-1.898263	-3.223223	-1.740456
H	-2.926823	-2.952500	-0.326919

MP2/6311G optimized geometry, all-*gauche*-Si_8Me_{18}**

80

RI-MP2
Energy= -3028.54934463936752
TD B3LYP
Energy= -3035.03452296

Si	-1.793235	1.784807	0.705012
H	-1.861945	4.077176	3.315525
H	-0.860521	7.274589	0.644366
H	-2.757467	5.510541	-1.086463
H	1.026962	3.692631	-2.110439
C	-1.853546	0.751301	2.300340
Si	-0.602340	3.760281	1.176696
C	-3.571472	2.312004	0.280510
H	0.880592	6.923286	0.711211
H	-1.797002	5.978154	-2.501918
C	-1.892966	5.240224	-1.699914
C	1.077819	3.379930	1.976298
Si	-0.318690	5.211669	-0.655561
C	-1.669759	4.703140	2.439006
H	0.174859	7.649470	-0.745416
H	-2.079169	4.265388	-2.155346
H	-2.628238	4.992667	1.998321
H	-4.205806	1.430219	0.149693
H	-3.597121	2.897465	-0.642212
H	-3.992791	2.916217	1.089272
H	-0.856783	0.649920	2.730026
H	-2.261576	-0.243582	2.101873
H	-2.492876	1.244636	3.038800
H	1.376844	5.389704	-2.465177
H	-1.151776	5.607523	2.771756
Si	-1.096308	0.430624	-1.092159
H	1.774542	2.959518	1.251871
H	0.956148	2.670895	2.800228
H	1.515772	4.299314	2.376706
C	0.000000	6.932363	0.062116
C	1.187033	4.672743	-1.660885
H	2.077561	4.624450	-1.027376
Si	1.096308	-0.430624	-1.092159
C	-1.278017	1.436095	-2.697238
C	-2.333521	-1.008285	-1.217427
H	2.284301	1.642270	-0.333746
C	2.333521	1.008285	-1.217427

H	2.119590	1.611779	-2.103165
C	1.278017	-1.436095	-2.697238
H	3.353059	0.622295	-1.309906
Si	1.793235	-1.784807	0.705012
H	-3.353059	-0.622295	-1.309906
H	-2.284301	-1.642270	-0.333746
H	-2.119590	-1.611779	-2.103165
H	-2.292448	1.836471	-2.780716
H	-1.094243	0.794784	-3.564538
H	-0.568875	2.263761	-2.726099
H	1.094243	-0.794784	-3.564538
H	0.568875	-2.263761	-2.726099
H	2.292448	-1.836471	-2.780716
H	1.861945	-4.077176	3.315525
H	0.860521	-7.274589	0.644366
H	2.757467	-5.510541	-1.086463
H	-1.026962	-3.692631	-2.110439
C	1.853546	-0.751301	2.300340
Si	0.602340	-3.760281	1.176696
C	3.571472	-2.312004	0.280510
H	-0.880592	-6.923286	0.711211
H	1.797002	-5.978154	-2.501918
C	1.892966	-5.240224	-1.699914
C	-1.077819	-3.379930	1.976298
Si	0.318690	-5.211669	-0.655561
C	1.669759	-4.703140	2.439006
H	-0.174859	-7.649470	-0.745416
H	2.079169	-4.265388	-2.155346
H	2.628238	-4.992667	1.998321
H	4.205806	-1.430219	0.149693
H	3.597121	-2.897465	-0.642212
H	3.992791	-2.916217	1.089272
H	0.856783	-0.649920	2.730026
H	2.261576	0.243582	2.101873
H	2.492876	-1.244636	3.038800
H	-1.376844	-5.389704	-2.465177
H	1.151776	-5.607523	2.771756
H	-1.774542	-2.959518	1.251871
H	-0.956148	-2.670895	2.800228
H	-1.515772	-4.299314	2.376706
C	0.000000	-6.932363	0.062116
C	-1.187033	-4.672743	-1.660885
H	-2.077561	-4.624450	-1.027376

MP2/6311G optimized geometry, all-*anti*-Si_9Me_{20}**

89
RI-MP2
Energy= -3397.13490833014384
TD B3LYP
Energy= -3404.40704599

Si	0.000000	-7.845323	0.549568
Si	0.000000	-5.877089	-0.750629
Si	0.000000	-3.914293	0.559191
Si	0.000000	-1.957133	-0.762965
Si	0.000000	0.000000	0.548093
Si	0.000000	1.957133	-0.762965
Si	0.000000	3.914293	0.559191
Si	0.000000	5.877089	-0.750629
Si	0.000000	7.845323	0.549568
C	-1.537481	-7.966960	1.641491
C	0.000000	-9.321849	-0.634288
C	1.537481	-7.966960	1.641491
C	1.540338	-5.934498	-1.863171
C	-1.540338	-5.934498	-1.863171
C	1.541609	-3.924967	1.668555
C	-1.541609	-3.924967	1.668555
C	-1.541567	-1.974020	-1.872251
C	1.541567	-1.974020	-1.872251
C	-1.542295	0.000000	1.656702
C	1.542295	0.000000	1.656702
C	-1.541567	1.974020	-1.872251
C	1.541567	1.974020	-1.872251
C	-1.541609	3.924967	1.668555
C	1.541609	3.924967	1.668555
C	1.540338	5.934498	-1.863171
C	-1.540338	5.934498	-1.863171
C	1.537481	7.966960	1.641491
C	-1.537481	7.966960	1.641491
C	0.000000	9.321849	-0.634288
H	0.870927	9.497250	-1.136812
H	-2.462260	-3.901136	1.074623
H	2.462260	-3.901136	1.074623
H	2.456650	-7.863301	1.057147
H	-1.574549	-4.825568	2.290791
H	1.555482	-3.058539	2.337713
H	1.574549	-4.825568	2.290791
H	-1.555482	-3.058539	2.337713
H	1.573385	-8.939961	2.146250

H	-0.870927	-9.497250	-1.136812
H	0.870927	-9.497250	-1.136812
H	1.547367	-7.193380	2.416523
H	0.000000	-10.266667	-0.078274
H	-1.547367	-7.193380	2.416523
H	-2.456650	-7.863301	1.057147
H	-1.573385	-8.939961	2.146250
H	1.590436	-6.880673	-2.413146
H	-2.461788	-5.841159	-1.280248
H	-1.531481	-5.125995	-2.601571
H	-1.590436	-6.880673	-2.413146
H	2.461788	-5.841159	-1.280248
H	1.531481	-5.125995	-2.601571
H	-2.461788	5.841159	-1.280248
H	2.461788	5.841159	-1.280248
H	-1.590436	6.880673	-2.413146
H	1.531481	5.125995	-2.601571
H	1.590436	6.880673	-2.413146
H	-1.531481	5.125995	-2.601571
H	1.573385	8.939961	2.146250
H	-2.456650	7.863301	1.057147
H	-1.547367	7.193380	2.416523
H	-1.573385	8.939961	2.146250
H	2.456650	7.863301	1.057147
H	1.547367	7.193380	2.416523
H	2.462303	-1.947017	-1.278462
H	-2.462303	-1.947017	-1.278462
H	-1.555398	-1.111399	-2.546310
H	-1.573452	-2.878211	-2.490063
H	1.573452	-2.878211	-2.490063
H	1.555536	-0.838218	2.331438
H	1.555398	-1.111399	-2.546310
H	-2.462165	0.000000	1.063591
H	-1.555536	-0.838218	2.331438
H	-1.555536	0.838218	2.331438
H	2.462165	0.000000	1.063591
H	1.555536	0.838218	2.331438
H	2.462260	3.901136	1.074623
H	-2.462260	3.901136	1.074623
H	-1.555482	3.058539	2.337713
H	-1.574549	4.825568	2.290791
H	1.574549	4.825568	2.290791
H	1.573452	2.878211	-2.490063
H	1.555482	3.058539	2.337713
H	-2.462303	1.947017	-1.278462

H	-1.573452	2.878211	-2.490063
H	-1.555398	1.111399	-2.546310
H	2.462303	1.947017	-1.278462
H	1.555398	1.111399	-2.546310
H	0.000000	10.266667	-0.078274
H	-0.870927	9.497250	-1.136812

MP2/6311G optimized geometry, all-*transoid*-Si_9Me_{20}**

89
RI-MP2
Energy= -3397.14873043656144
TD B3LYP
Energy= -3404.41311964

Si	1.681077	7.540841	0.308161
Si	2.104224	5.392557	-0.554888
Si	0.801537	3.774716	0.551878
Si	0.712263	1.791548	-0.710953
Si	0.000000	0.000000	0.629846
Si	-0.712263	-1.791548	-0.710953
Si	-0.801537	-3.774716	0.551878
Si	-2.104224	-5.392557	-0.554888
Si	-1.681077	-7.540841	0.308161
C	1.685479	7.517724	2.198415
C	3.014797	8.745038	-0.281472
C	0.000000	8.159999	-0.292688
C	3.939571	4.966327	-0.311855
C	1.731129	5.403765	-2.418418
C	1.582510	3.438189	2.250733
C	-0.968967	4.410584	0.816374
C	-0.486230	1.984407	-2.172251
C	2.448954	1.440499	-1.396477
C	1.405229	-0.605846	1.741115
C	-1.405229	0.605846	1.741115
C	-2.448954	-1.440499	-1.396477
C	0.486230	-1.984407	-2.172251
C	0.968967	-4.410584	0.816374
C	-1.582510	-3.438189	2.250733
C	-1.731129	-5.403765	-2.418418
C	-3.939571	-4.966327	-0.311855
C	-1.685479	-7.517724	2.198415
C	0.000000	-8.159999	-0.292688
C	-3.014797	-8.745038	-0.281472
H	-2.657024	-9.796275	-0.050538
H	-3.936660	-8.600839	0.265486
H	2.285033	-0.884710	1.151266
H	2.441837	0.571501	-2.063881
H	1.711708	0.172423	2.448930
H	1.105841	-1.483639	2.324511
H	2.830133	2.293503	-1.968832
H	3.163093	1.236286	-0.591461
H	-0.135887	2.752787	-2.870778

H	-0.582554	1.048067	-2.732536
H	-1.487161	2.273477	-1.834077
H	-1.105841	1.483639	2.324511
H	-2.285033	0.884710	1.151266
H	-1.711708	-0.172423	2.448930
H	1.435683	-4.648671	-0.127742
H	0.135887	-2.752787	-2.870778
H	1.533150	-3.794944	1.418809
H	0.883369	-5.437744	1.354835
H	0.582554	-1.048067	-2.732536
H	1.487161	-2.273477	-1.834077
H	-2.441837	-0.571501	-2.063881
H	-2.830133	-2.293503	-1.968832
H	-3.163093	-1.236286	-0.591461
H	-1.029525	-2.579222	2.751430
H	-2.625305	-3.047279	2.150117
H	-1.572503	-4.254770	2.901118
H	2.657024	9.796275	-0.050538
H	4.174013	3.970155	-0.702115
H	3.059396	8.791478	-1.374902
H	4.215012	4.980875	0.748080
H	0.881503	6.888169	2.594461
H	1.541796	8.527323	2.601013
H	2.632535	7.136384	2.595287
H	-1.533150	3.794944	1.418809
H	-1.435683	4.648671	-0.127742
H	-0.883369	5.437744	1.354835
H	2.625305	3.047279	2.150117
H	1.029525	2.579222	2.751430
H	1.572503	4.254770	2.901118
H	-0.035922	8.215633	-1.385897
H	3.936660	8.600839	0.265486
H	0.670191	5.590743	-2.616120
H	1.993263	4.446767	-2.882770
H	2.305324	6.184969	-2.929975
H	4.581571	5.686525	-0.831408
H	-0.207559	9.163801	0.096032
H	-0.812673	7.502912	0.033122
H	0.812673	-7.502912	0.033122
H	0.035922	-8.215633	-1.385897
H	-4.174013	-3.970155	-0.702115
H	-4.215012	-4.980875	0.748080
H	-4.581571	-5.686525	-0.831408
H	-0.670191	-5.590743	-2.616120
H	-1.993263	-4.446767	-2.882770

H	-2.305324	-6.184969	-2.929975
H	-2.632535	-7.136384	2.595287
H	-0.881503	-6.888169	2.594461
H	-1.541796	-8.527323	2.601013
H	0.207559	-9.163801	0.096032

MP2/6311G optimized geometry, all-*deviant*-Si_9Me_{20}**

89
RI-MP2
Energy= -3397.15045261104524
TD B3LYP
Energy= -3404.41681139

Si	0.000000	7.749986	-0.094669
Si	1.232812	5.741163	-0.108516
Si	-0.161883	3.922153	0.468311
Si	0.499094	1.908195	-0.575447
Si	0.000000	0.000000	0.735704
Si	-0.499094	-1.908195	-0.575447
Si	0.161883	-3.922153	0.468311
Si	-1.232812	-5.741163	-0.108516
Si	0.000000	-7.749986	-0.094669
C	-1.228908	7.757282	-1.538772
C	1.177216	9.224017	-0.310579
C	-0.948279	7.978521	1.532624
C	2.677727	5.810517	1.130963
C	1.963577	5.588423	-1.865555
C	-1.981067	4.220057	-0.019039
C	-0.083478	3.818157	2.372099
C	2.371241	1.857340	-0.933446
C	-0.410382	1.894419	-2.252957
C	-1.538216	0.250581	1.828047
C	1.538216	-0.250581	1.828047
C	-2.371241	-1.857340	-0.933446
C	0.410382	-1.894419	-2.252957
C	0.083478	-3.818157	2.372099
C	1.981067	-4.220057	-0.019039
C	-2.677727	-5.810517	1.130963
C	-1.963577	-5.588423	-1.865555
C	1.228908	-7.757282	-1.538772
C	0.948279	-7.978521	1.532624
C	-1.177216	-9.224017	-0.310579
H	-0.675147	-10.169345	-0.544192
H	-1.871344	-9.062426	-1.290419
H	2.316434	5.957340	2.164505
H	-1.494431	8.940631	1.533314
H	1.894299	9.289220	0.527704
H	0.675147	10.169345	-0.544192
H	-1.685351	7.169936	1.687458
H	-0.259249	7.980035	2.396938
H	-2.386354	5.113695	0.489921

H	-2.601358	3.352161	0.274419
H	-2.092858	4.364784	-1.108461
H	1.871344	9.062426	-1.290419
H	3.361025	6.644251	0.884361
H	3.262520	4.872168	1.103474
H	-0.289188	4.808357	2.820284
H	0.914061	3.490757	2.717022
H	-0.832699	3.107594	2.762964
H	-1.785440	8.713087	-1.564833
H	-1.962342	6.936855	-1.449328
H	-0.704662	7.644403	-2.505122
H	2.497933	6.516170	-2.143461
H	1.171024	5.415709	-2.616195
H	2.683326	4.753709	-1.930786
H	0.704662	-7.644403	-2.505122
H	-3.361025	-6.644251	0.884361
H	-3.262520	-4.872168	1.103474
H	-2.316434	-5.957340	2.164505
H	1.785440	-8.713087	-1.564833
H	1.962342	-6.936855	-1.449328
H	-2.497933	-6.516170	-2.143461
H	-1.171024	-5.415709	-2.616195
H	-2.683326	-4.753709	-1.930786
H	1.494431	-8.940631	1.533314
H	0.259249	-7.980035	2.396938
H	1.685351	-7.169936	1.687458
H	-2.410460	0.565914	1.227215
H	-0.042748	1.077391	-2.898184
H	-1.359975	1.016130	2.603399
H	-1.802101	-0.694395	2.338997
H	-0.245909	2.848768	-2.787603
H	-1.499645	1.764060	-2.119702
H	2.668828	2.683511	-1.604840
H	2.638928	0.904827	-1.428609
H	2.966010	1.937060	-0.005989
H	1.802101	0.694395	2.338997
H	2.410460	-0.565914	1.227215
H	1.359975	-1.016130	2.603399
H	-0.914061	-3.490757	2.717022
H	-2.668828	-2.683511	-1.604840
H	0.832699	-3.107594	2.762964
H	0.289188	-4.808357	2.820284
H	-2.638928	-0.904827	-1.428609
H	-2.966010	-1.937060	-0.005989
H	0.042748	-1.077391	-2.898184

H	0.245909	-2.848768	-2.787603
H	1.499645	-1.764060	-2.119702
H	2.601358	-3.352161	0.274419
H	2.092858	-4.364784	-1.108461
H	2.386354	-5.113695	0.489921
H	-1.894299	-9.289220	0.527704

MP2/6311G optimized geometry, all-*eclipsed*-Si_9Me_{20}**

89
RI-MP2
Energy= -3397.11681565832350
TD B3LYP
Energy= -3404.38678233

Si	1.665080	7.481939	-0.669062
Si	1.464589	5.637946	0.789665
Si	0.000000	3.951087	-0.034059
Si	0.959641	1.793213	-0.369208
Si	0.000000	0.000000	0.882400
Si	-0.959641	-1.793213	-0.369208
Si	0.000000	-3.951087	-0.034059
Si	-1.464589	-5.637946	0.789665
Si	-1.665080	-7.481939	-0.669062
C	2.864720	8.724435	0.121223
C	0.006896	8.363246	-0.933596
C	2.379681	6.969217	-2.349330
C	3.232679	5.042985	1.182589
C	0.733189	6.271957	2.435929
C	-1.501459	3.934263	1.140776
C	-0.705081	4.462464	-1.733957
C	0.939728	1.491922	-2.251686
C	2.808152	1.811613	0.111382
C	1.400439	-0.640456	2.005967
C	-1.400439	0.640456	2.005967
C	-2.808152	-1.811613	0.111382
C	-0.939728	-1.491922	-2.251686
C	0.705081	-4.462464	-1.733957
C	1.501459	-3.934263	1.140776
C	-3.232679	-5.042985	1.182589
C	-0.733189	-6.271957	2.435929
C	-0.006896	-8.363246	-0.933596
C	-2.379681	-6.969217	-2.349330
C	-2.864720	-8.724435	0.121223
H	-2.979840	-9.685208	-0.595356
H	-2.597501	-9.214945	1.087556
H	0.151756	9.268536	-1.552713
H	3.867330	8.281404	0.260501
H	-0.431798	8.679274	0.030276
H	1.699476	6.287568	-2.889697
H	-0.725033	7.715146	-1.446802
H	2.543890	7.860350	-2.983945
H	3.769135	4.706824	0.278378

H	3.226139	4.207131	1.904803
H	3.806056	5.875453	1.631321
H	-0.277957	6.694410	2.298009
H	1.379318	7.061723	2.862531
H	0.660877	5.455856	3.178538
H	-1.225279	3.656524	2.172340
H	-2.269279	3.222990	0.787292
H	-1.957811	4.941178	1.169201
H	0.084269	4.556357	-2.499688
H	-1.227761	5.433121	-1.657765
H	-1.434996	3.711822	-2.089539
H	2.979840	9.685208	-0.595356
H	3.351904	6.457850	-2.226917
H	2.597501	9.214945	1.087556
H	0.431798	-8.679274	0.030276
H	0.725033	-7.715146	-1.446802
H	-0.151756	-9.268536	-1.552713
H	-3.351904	-6.457850	-2.226917
H	-2.543890	-7.860350	-2.983945
H	-1.699476	-6.287568	-2.889697
H	-3.769135	-4.706824	0.278378
H	-3.226139	-4.207131	1.904803
H	-3.806056	-5.875453	1.631321
H	0.277957	-6.694410	2.298009
H	-1.379318	-7.061723	2.862531
H	-0.660877	-5.455856	3.178538
H	-2.257193	0.969502	1.548736
H	3.271535	0.830915	-0.103531
H	-1.000368	1.362082	2.758083
H	-1.701091	-0.281195	2.697533
H	-0.083987	1.465251	-2.662581
H	2.257193	-0.969502	1.548736
H	1.435547	0.537049	-2.502266
H	1.490369	2.304934	-2.760360
H	2.956338	2.028428	1.183420
H	3.350201	2.577283	-0.472660
H	1.000368	-1.362082	2.758083
H	1.701091	0.281195	2.697533
H	1.225279	-3.656524	2.172340
H	-1.490369	-2.304934	-2.760360
H	2.269279	-3.222990	0.787292
H	1.957811	-4.941178	1.169201
H	-2.956338	-2.028428	1.183420
H	-0.084269	-4.556357	-2.499688
H	-3.350201	-2.577283	-0.472660

H	-3.271535	-0.830915	-0.103531
H	0.083987	-1.465251	-2.662581
H	-1.435547	-0.537049	-2.502266
H	1.227761	-5.433121	-1.657765
H	1.434996	-3.711822	-2.089539
H	-3.867330	-8.281404	0.260501

MP2/6311G optimized geometry, all-*ortho*-Si_9Me_{20}**

89
RI-MP2
Energy= -3397.17122042859637
TD B3LYP
Energy= -3404.43469338

Si	-4.234148	5.501658	0.330238
Si	-4.152368	3.157977	0.568864
Si	-2.784700	2.089355	-1.029489
Si	-0.514705	1.915343	-0.407669
Si	0.000000	0.000000	0.871500
Si	0.514705	-1.915343	-0.407669
Si	2.784700	-2.089355	-1.029489
Si	4.152368	-3.157977	0.568864
Si	4.234148	-5.501658	0.330238
C	-2.513255	6.280020	0.192103
C	-5.264393	6.003840	-1.169434
C	-5.071089	6.216688	1.874607
C	-5.917249	2.481526	0.353805
C	-3.610862	2.737822	2.340418
C	-2.860569	3.064547	-2.661029
C	-3.520330	0.374011	-1.385330
C	0.000000	3.443719	0.598152
C	0.528168	1.931832	-1.996416
C	-1.461838	-0.432527	2.006321
C	1.461838	0.432527	2.006321
C	0.000000	-3.443719	0.598152
C	-0.528168	-1.931832	-1.996416
C	2.860569	-3.064547	-2.661029
C	3.520330	-0.374011	-1.385330
C	5.917249	-2.481526	0.353805
C	3.610862	-2.737822	2.340418
C	5.071089	-6.216688	1.874607
C	2.513255	-6.280020	0.192103
C	5.264393	-6.003840	-1.169434
H	6.300429	-5.710824	-1.031493
H	-1.982168	5.937399	-0.701961
H	-4.904938	5.555207	-2.093112
H	-1.893254	6.038507	1.061132
H	-5.184785	7.303438	1.792186
H	-4.482583	6.012870	2.775026
H	-2.590672	7.371691	0.133064
H	-6.300429	5.710824	-1.031493
H	-6.068610	5.790671	2.026841

H	-5.232572	7.085178	-1.294837
H	-6.296048	2.648384	-0.660178
H	-6.612639	2.961952	1.051620
H	-5.948279	1.403272	0.545249
H	-4.301245	3.180900	3.066732
H	-2.608431	3.116486	2.563801
H	-3.603172	1.656110	2.506967
H	-3.895735	3.191073	-2.998288
H	-2.316456	2.538244	-3.453345
H	-2.417986	4.061716	-2.562829
H	-4.543296	0.469240	-1.766560
H	-3.560010	-0.249170	-0.485872
H	-2.933548	-0.163972	-2.136919
H	0.269176	1.104078	-2.664656
H	1.597242	1.855588	-1.770471
H	0.371246	2.864090	-2.549882
H	-0.213393	4.368716	0.051945
H	1.075170	3.422177	0.807997
H	-0.522416	3.496454	1.558867
H	-2.345541	-0.738443	1.436989
H	-1.746555	0.421702	2.629778
H	-1.198230	-1.258983	2.675313
H	1.198230	1.258983	2.675313
H	2.345541	0.738443	1.436989
H	1.746555	-0.421702	2.629778
H	0.522416	-3.496454	1.558867
H	0.213393	-4.368716	0.051945
H	-1.075170	-3.422177	0.807997
H	-0.371246	-2.864090	-2.549882
H	-0.269176	-1.104078	-2.664656
H	-1.597242	-1.855588	-1.770471
H	3.560010	0.249170	-0.485872
H	2.933548	0.163972	-2.136919
H	4.543296	-0.469240	-1.766560
H	3.895735	-3.191073	-2.998288
H	2.316456	-2.538244	-3.453345
H	2.417986	-4.061716	-2.562829
H	6.612639	-2.961952	1.051620
H	5.948279	-1.403272	0.545249
H	6.296048	-2.648384	-0.660178
H	4.301245	-3.180900	3.066732
H	2.608431	-3.116486	2.563801
H	3.603172	-1.656110	2.506967
H	5.232572	-7.085178	-1.294837
H	6.068610	-5.790671	2.026841

H	5.184785	-7.303438	1.792186
H	4.482583	-6.012870	2.775026
H	2.590672	-7.371691	0.133064
H	1.982168	-5.937399	-0.701961
H	1.893254	-6.038507	1.061132
H	4.904938	-5.555207	-2.093112

MP2/6311G optimized geometry, all-*gauche*-Si_9Me_{20}**

89
RI-MP2
Energy= -3397.16512247888068
TD B3LYP
Energy= -3404.42610971

Si	0.000000	5.877534	1.197528
Si	-0.737398	4.629031	-0.656231
Si	0.704317	2.946782	-1.454631
Si	1.528580	1.336146	0.053838
Si	0.000000	0.000000	1.248573
Si	-1.528580	-1.336146	0.053838
Si	-0.704317	-2.946782	-1.454631
Si	0.737398	-4.629031	-0.656231
Si	0.000000	-5.877534	1.197528
C	-0.442005	4.991721	2.805043
C	-0.937819	7.516915	1.128291
C	1.843320	6.263335	1.117070
C	-2.461753	3.927544	-0.274262
C	-0.909860	5.861008	-2.095639
C	-0.189955	2.095827	-2.900255
C	2.240631	3.805170	-2.174569
C	2.678260	0.206488	-0.955695
C	2.618370	2.202422	1.349499
C	1.035556	-1.118553	2.386304
C	-1.035556	1.118553	2.386304
C	-2.618370	-2.202422	1.349499
C	-2.678260	-0.206488	-0.955695
C	0.189955	-2.095827	-2.900255
C	-2.240631	-3.805170	-2.174569
C	2.461753	-3.927544	-0.274262
C	0.909860	-5.861008	-2.095639
C	0.937819	-7.516915	1.128291
C	0.442005	-4.991721	2.805043
C	-1.843320	-6.263335	1.117070
H	0.227566	-5.638352	3.656368
H	-2.405692	-5.393339	1.348742
H	-2.115130	-6.631424	0.146837
H	-1.577919	0.518127	3.110384
H	-1.756361	1.686946	1.818081
H	-0.396867	1.802384	2.931514
H	0.396867	-1.802384	2.931514
H	1.577919	-0.518127	3.110384
H	1.756361	-1.686946	1.818081

H	2.198115	-0.096223	-1.885792
H	2.950061	-0.683434	-0.382325
H	3.596783	0.744160	-1.209768
H	3.108376	1.459665	1.986018
H	2.025264	2.860417	1.983402
H	3.396035	2.790652	0.855678
H	-3.108376	-1.459665	1.986018
H	-2.025264	-2.860417	1.983402
H	-3.396035	-2.790652	0.855678
H	-2.950061	0.683434	-0.382325
H	-3.596783	-0.744160	-1.209768
H	-2.198115	0.096223	-1.885792
H	2.886103	3.070367	-2.663869
H	2.815834	4.302313	-1.392380
H	1.946247	4.549261	-2.920099
H	-1.211430	1.838083	-2.622578
H	0.341903	1.191883	-3.206382
H	-0.235203	2.773711	-3.758033
H	1.211430	-1.838083	-2.622578
H	-0.341903	-1.191883	-3.206382
H	0.235203	-2.773711	-3.758033
H	-2.886103	-3.070367	-2.663869
H	-2.815834	-4.302313	-1.392380
H	-1.946247	-4.549261	-2.920099
H	-1.289948	5.351311	-2.985281
H	0.054072	6.314270	-2.339434
H	-1.612706	6.656822	-1.832704
H	-2.461120	3.378350	0.662560
H	-2.791475	3.265453	-1.074339
H	-3.183267	4.741522	-0.186591
H	1.289948	-5.351311	-2.985281
H	-0.054072	-6.314270	-2.339434
H	1.612706	-6.656822	-1.832704
H	2.461120	-3.378350	0.662560
H	2.791475	-3.265453	-1.074339
H	3.183267	-4.741522	-0.186591
H	-0.680977	8.073534	0.222949
H	2.115130	6.631424	0.146837
H	0.133979	4.077924	2.920332
H	-2.016276	7.339835	1.136884
H	2.065492	7.015081	1.836584
H	-0.684545	8.132847	1.994608
H	2.405692	5.393339	1.348742
H	-0.227566	5.638352	3.656368
H	-1.504022	4.738667	2.826837

H	-2.065492	-7.015081	1.836584
H	2.016276	-7.339835	1.136884
H	0.680977	-8.073534	0.222949
H	0.684545	-8.132847	1.994608
H	-0.133979	-4.077924	2.920332
H	1.504022	-4.738667	2.826837

MP2/6311G optimized geometry, all-*anti*-$Si_{10}Me_{22}$**

98
RI-MP2
Energy= -3765.79103296404082
TD B3LYP
Energy= -3773.83717226

H	1.174314	-4.890634	2.462000
H	1.174314	-4.890634	-2.462000
C	1.729472	-8.958023	1.537000
H	1.144546	-8.852614	-2.457000
Si	0.637559	-8.833260	0.000000
C	-0.550470	-10.306430	0.000000
C	1.729472	-8.958023	-1.537000
H	2.387666	-5.818482	1.574000
H	2.438901	-4.051517	-1.556000
H	2.387666	-5.818482	-1.574000
H	2.438901	-4.051517	1.556000
H	2.230792	-9.932373	-1.574000
H	-1.197468	-10.302978	0.884000
H	-1.197468	-10.302978	-0.884000
H	2.506012	-8.186565	-1.548000
H	0.002868	-11.252817	0.000000
H	2.506012	-8.186565	1.548000
H	1.144546	-8.852614	2.457000
H	2.230792	-9.932373	1.574000
Si	-0.658306	-2.941379	0.000000
H	-2.322762	-7.860191	-1.590000
H	-1.186037	-6.823985	2.462000
Si	0.658306	-4.902273	0.000000
H	-2.505535	-6.105063	1.532000
H	-2.322762	-7.860191	1.590000
H	-1.186037	-6.823985	-2.462000
H	-2.505535	-6.105063	-1.532000
C	1.767297	-4.916048	-1.542000
C	1.767297	-4.916048	1.542000
Si	-0.657063	-6.861354	0.000000
C	-1.770101	-6.915577	-1.540000
C	-1.770101	-6.915577	1.540000
H	-1.174314	4.890634	2.462000
H	-1.174314	4.890634	-2.462000
C	-1.729472	8.958023	1.537000
H	-1.144546	8.852614	-2.457000
Si	-0.637559	8.833260	0.000000
C	0.550470	10.306430	0.000000

C	-1.729472	8.958023	-1.537000
H	-2.387666	5.818482	1.574000
H	-2.438901	4.051517	-1.556000
H	-2.387666	5.818482	-1.574000
H	-2.438901	4.051517	1.556000
H	-2.230792	9.932373	-1.574000
H	1.197468	10.302978	0.884000
H	1.197468	10.302978	-0.884000
H	-2.506012	8.186565	-1.548000
H	-0.002868	11.252817	0.000000
H	-2.506012	8.186565	1.548000
H	-1.144546	8.852614	2.457000
H	-2.230792	9.932373	1.574000
Si	0.658306	2.941379	0.000000
H	2.322762	7.860191	-1.590000
H	1.186037	6.823985	2.462000
Si	-0.658306	4.902273	0.000000
H	2.505535	6.105063	1.532000
H	2.322762	7.860191	1.590000
H	1.186037	6.823985	-2.462000
H	2.505535	6.105063	-1.532000
C	-1.767297	4.916048	-1.542000
C	-1.767297	4.916048	1.542000
Si	0.657063	6.861354	0.000000
C	1.770101	6.915577	-1.540000
C	1.770101	6.915577	1.540000
H	-1.174314	-2.929745	-2.462000
C	1.767297	-0.966662	1.542000
H	-1.174314	-2.929745	2.462000
C	1.767297	-0.966662	-1.542000
Si	0.658306	-0.980447	0.000000
H	-2.438909	-2.090640	1.556000
H	-2.387658	-3.857604	1.574000
H	-2.387658	-3.857604	-1.574000
H	2.438909	-1.831187	-1.556000
H	-2.438909	-2.090640	-1.556000
H	1.174314	-0.992082	2.462000
H	2.438909	-1.831187	1.556000
C	-1.767297	-2.955164	1.542000
H	2.387658	-0.064222	1.574000
H	1.174314	-0.992082	-2.462000
C	-1.767297	-2.955164	-1.542000
H	2.387658	-0.064222	-1.574000
Si	-0.658306	0.980447	0.000000
H	1.174314	2.929745	-2.462000

C	-1.767297	0.966662	1.542000
H	1.174314	2.929745	2.462000
C	-1.767297	0.966662	-1.542000
H	2.438909	2.090640	1.556000
H	2.387658	3.857604	1.574000
H	2.387658	3.857604	-1.574000
H	-2.438909	1.831187	-1.556000
H	2.438909	2.090640	-1.556000
H	-1.174314	0.992082	2.462000
H	-2.438909	1.831187	1.556000
C	1.767297	2.955164	1.542000
H	-2.387658	0.064222	1.574000
H	-1.174314	0.992082	-2.462000
C	1.767297	2.955164	-1.542000
H	-2.387658	0.064222	-1.574000

MP2/6311G optimized geometry, all-*transoid*-$Si_{10}Me_{22}$**

98
RI-MP2
Energy= -3765.79955592722717
TD B3LYP
Energy= -3773.83796396

Si	-0.021903	1.176196	0.008048
Si	2.144290	2.035465	0.331981
C	3.368169	1.010770	-0.698112
C	2.637179	1.904179	2.162036
H	-0.781519	1.473005	2.387974
C	-1.173908	1.752795	1.404362
H	2.696250	0.857558	2.480988
C	-0.698244	1.830963	-1.642048
H	-1.295541	2.841684	1.391648
H	-2.170411	1.307910	1.306568
H	3.616589	2.360612	2.343499
Si	0.021903	-1.176196	0.008048
Si	2.228990	4.301036	-0.297050
H	1.911683	2.409024	2.808977
H	4.401481	1.322154	-0.507338
H	3.294644	-0.055177	-0.456698
H	3.179815	1.121909	-1.771405
H	-0.666822	2.925355	-1.677370
H	-0.117221	1.454528	-2.490867
H	-1.740283	1.525475	-1.790105
Si	-2.144290	-2.035465	0.331981
C	0.698244	-1.830963	-1.642048
C	1.173908	-1.752795	1.404362
H	-1.911683	-2.409024	2.808977
C	-2.637179	-1.904179	2.162036
H	1.295541	-2.841684	1.391648
C	-3.368169	-1.010770	-0.698112
H	-2.696250	-0.857558	2.480988
H	-3.616589	-2.360612	2.343499
H	2.170411	-1.307910	1.306568
Si	-2.228990	-4.301036	-0.297050
H	0.781519	-1.473005	2.387974
H	1.740283	-1.525475	-1.790105
H	0.666822	-2.925355	-1.677370
H	0.117221	-1.454528	-2.490867
H	-3.294644	0.055177	-0.456698
H	-3.179815	-1.121909	-1.771405
H	-4.401481	-1.322154	-0.507338

C	3.047417	8.381879	-0.720658
C	5.876587	8.351159	0.470174
H	6.132640	9.280468	-0.052018
H	3.616807	4.768273	2.995357
C	0.698244	5.221206	0.350546
Si	4.146280	5.329239	0.600800
C	2.240594	4.408268	-2.193715
C	5.336492	6.985349	-2.226909
H	6.805820	7.791719	0.622775
H	2.995877	6.370670	2.579341
C	5.658963	4.188131	0.453379
Si	4.615668	7.345980	-0.517888
C	3.839861	5.686417	2.441388
H	2.308192	7.873162	-1.348608
H	3.274497	9.344582	-1.193583
H	2.574964	8.592360	0.244913
H	1.383830	3.880169	-2.626147
H	3.150086	3.966041	-2.614481
H	2.190498	5.450120	-2.530054
H	0.598216	5.116699	1.436279
H	-0.218632	4.833487	-0.107326
H	0.753116	6.291920	0.124571
H	6.264856	6.408938	-2.153552
H	5.486905	8.622117	1.457023
H	5.849701	3.903804	-0.587013
H	5.520972	3.267393	1.030770
H	6.561949	4.680861	0.832197
H	4.719995	6.147847	2.903159
H	5.567071	7.916629	-2.757338
H	4.638919	6.413592	-2.847262
C	-3.047417	-8.381879	-0.720658
C	-5.876587	-8.351159	0.470174
H	-6.132640	-9.280468	-0.052018
H	-3.616807	-4.768273	2.995357
C	-0.698244	-5.221206	0.350546
Si	-4.146280	-5.329239	0.600800
C	-2.240594	-4.408268	-2.193715
C	-5.336492	-6.985349	-2.226909
H	-6.805820	-7.791719	0.622775
H	-2.995877	-6.370670	2.579341
C	-5.658963	-4.188131	0.453379
Si	-4.615668	-7.345980	-0.517888
C	-3.839861	-5.686417	2.441388
H	-2.308192	-7.873162	-1.348608
H	-3.274497	-9.344582	-1.193583

H	-2.574964	-8.592360	0.244913
H	-1.383830	-3.880169	-2.626147
H	-3.150086	-3.966041	-2.614481
H	-2.190498	-5.450120	-2.530054
H	-0.598216	-5.116699	1.436279
H	0.218632	-4.833487	-0.107326
H	-0.753116	-6.291920	0.124571
H	-6.264856	-6.408938	-2.153552
H	-5.486905	-8.622117	1.457023
H	-5.849701	-3.903804	-0.587013
H	-5.520972	-3.267393	1.030770
H	-6.561949	-4.680861	0.832197
H	-4.719995	-6.147847	2.903159
H	-5.567071	-7.916629	-2.757338
H	-4.638919	-6.413592	-2.847262

MP2/6311G optimized geometry, all-*deviant*-$Si_{10}Me_{22}$**

98
RI-MP2
Energy= -3765.78667895292529
TD B3LYP
Energy= -3773.82739989

H	-2.561485	7.071636	1.346148
Si	-0.379827	4.849188	-0.514552
C	0.486733	4.989229	-2.207227
C	-2.256524	4.720626	-0.835257
Si	-0.109763	6.796545	0.797535
C	1.820493	8.605180	-1.476972
H	-1.119931	9.707619	-2.500231
H	-0.862459	10.378702	0.978219
Si	0.146673	8.684894	-0.589463
C	-1.629750	6.975604	1.931764
C	1.449522	6.740297	1.897534
H	0.269645	11.156481	-0.166841
H	-1.234814	7.924562	-2.555736
H	-2.230895	8.848450	-1.394856
H	0.079023	5.833761	-2.792398
H	0.330391	4.063878	-2.793236
H	1.575237	5.141587	-2.096646
H	0.901517	10.247373	1.236627
H	-1.532772	7.871855	2.572193
H	-1.730914	6.094693	2.592822
C	0.109763	10.262949	0.465812
C	-1.239067	8.799096	-1.880287
Si	0.492207	2.921289	0.536691
H	-2.647332	5.680415	-1.222238
H	-2.808063	4.479177	0.091433
H	-2.479933	3.938616	-1.581953
H	1.967963	9.506936	-2.100718
H	1.887804	7.720288	-2.133829
H	2.651794	8.556577	-0.750347
H	1.609255	7.717196	2.391130
H	2.351985	6.509175	1.302912
H	1.356623	5.975443	2.688362
H	2.561485	-7.071636	1.346148
Si	0.379827	-4.849188	-0.514552
C	-0.486733	-4.989229	-2.207227
C	2.256524	-4.720626	-0.835257
Si	0.109763	-6.796545	0.797535
C	-1.820493	-8.605180	-1.476972

H	1.119931	-9.707619	-2.500231
H	0.862459	-10.378702	0.978219
Si	-0.146673	-8.684894	-0.589463
C	1.629750	-6.975604	1.931764
C	-1.449522	-6.740297	1.897534
H	-0.269645	-11.156481	-0.166841
H	1.234814	-7.924562	-2.555736
H	2.230895	-8.848450	-1.394856
H	-0.079023	-5.833761	-2.792398
H	-0.330391	-4.063878	-2.793236
H	-1.575237	-5.141587	-2.096646
H	-0.901517	-10.247373	1.236627
H	1.532772	-7.871855	2.572193
H	1.730914	-6.094693	2.592822
C	-0.109763	-10.262949	0.465812
C	1.239067	-8.799096	-1.880287
Si	-0.492207	-2.921289	0.536691
H	2.647332	-5.680415	-1.222238
H	2.808063	-4.479177	0.091433
H	2.479933	-3.938616	-1.581953
H	-1.967963	-9.506936	-2.100718
H	-1.887804	-7.720288	-2.133829
H	-2.651794	-8.556577	-0.750347
H	-1.609255	-7.717196	2.391130
H	-2.351985	-6.509175	1.302912
H	-1.356623	-5.975443	2.688362
Si	-0.688730	0.959812	-0.046528
C	0.440757	3.046303	2.438640
C	2.325536	2.853469	0.011639
H	-0.649373	1.290712	-2.554398
C	-1.424010	1.045610	-1.805327
H	2.874640	2.084108	0.582231
C	-2.141242	0.810176	1.179645
H	-2.217289	1.810973	-1.868056
H	-1.869359	0.072130	-2.084045
H	2.815351	3.827676	0.197868
Si	0.688730	-0.959812	-0.046528
H	2.428296	2.622731	-1.064207
H	1.035258	3.907244	2.795341
H	0.864289	2.130447	2.892459
H	-0.592330	3.163925	2.811708
H	-2.765801	1.722741	1.143947
H	-1.786713	0.681444	2.217922
H	-2.785801	-0.051585	0.927061
C	2.141242	-0.810176	1.179645

C	1.424010	-1.045610	-1.805327
H	-2.428296	-2.622731	-1.064207
C	-2.325536	-2.853469	0.011639
H	2.217289	-1.810973	-1.868056
C	-0.440757	-3.046303	2.438640
H	-2.874640	-2.084108	0.582231
H	-2.815351	-3.827676	0.197868
H	1.869359	-0.072130	-2.084045
H	0.649373	-1.290712	-2.554398
H	2.785801	0.051585	0.927061
H	2.765801	-1.722741	1.143947
H	1.786713	-0.681444	2.217922
H	-0.864289	-2.130447	2.892459
H	0.592330	-3.163925	2.811708
H	-1.035258	-3.907244	2.795341

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{10}Me_{22}$**

98
RI-MP2
Energy= -3765.76705517025175
TD B3LYP
Energy= -3773.81074226

Si	-8.342692	-2.278119	-0.421037
Si	-6.797480	-0.556177	0.043323
Si	-4.666351	-1.372522	0.722226
H	-9.482356	-4.090499	0.874864
H	-9.845490	-0.864241	-1.868685
C	-9.976595	-1.469117	-0.953350
C	-6.768884	0.592528	-1.477915
C	-7.495265	0.481588	1.486667
C	-4.460787	-0.861088	2.547350
C	-4.666351	-3.282504	0.738541
H	-9.047887	-2.730105	1.949193
H	-6.828538	-3.931878	-1.574876
H	-7.796394	-3.899220	1.435167
H	-8.526399	-4.129604	-2.098070
H	-6.432626	0.068031	-2.389079
H	-6.101445	1.458050	-1.317649
H	-7.788601	0.979112	-1.661911
H	-7.604840	-0.119681	2.406652
H	-8.489790	0.886069	1.221116
H	-6.832789	1.336295	1.717577
H	-4.451661	0.234448	2.678710
H	-3.521449	-1.265130	2.965446
H	-5.300311	-1.268778	3.140587
H	-4.829037	-3.706349	-0.267502
H	-5.462386	-3.661837	1.404580
H	-3.699310	-3.664234	1.115094
H	-10.738793	-2.243036	-1.163999
H	-7.542625	-2.787620	-2.749416
H	-10.374313	-0.808496	-0.161725
C	-8.694435	-3.348615	1.104272
C	-7.749523	-3.384636	-1.842518
Si	-2.814138	-0.750489	-0.645999
Si	8.342692	2.278119	-0.421037
Si	6.797480	0.556177	0.043323
Si	4.666351	1.372522	0.722226
H	9.482356	4.090499	0.874864
H	9.845490	0.864241	-1.868685
C	9.976595	1.469117	-0.953350

C	6.768884	-0.592528	-1.477915
C	7.495265	-0.481588	1.486667
C	4.460787	0.861088	2.547350
C	4.666351	3.282504	0.738541
H	9.047887	2.730105	1.949193
H	6.828538	3.931878	-1.574876
H	7.796394	3.899220	1.435167
H	8.526399	4.129604	-2.098070
H	6.432626	-0.068031	-2.389079
H	6.101445	-1.458050	-1.317649
H	7.788601	-0.979112	-1.661911
H	7.604840	0.119681	2.406652
H	8.489790	-0.886069	1.221116
H	6.832789	-1.336295	1.717577
H	4.451661	-0.234448	2.678710
H	3.521449	1.265130	2.965446
H	5.300311	1.268778	3.140587
H	4.829037	3.706349	-0.267502
H	5.462386	3.661837	1.404580
H	3.699310	3.664234	1.115094
H	10.738793	2.243036	-1.163999
H	7.542625	2.787620	-2.749416
H	10.374313	0.808496	-0.161725
C	8.694435	3.348615	1.104272
C	7.749523	3.384636	-1.842518
Si	2.814138	0.750489	-0.645999
H	-1.521353	0.019650	2.881128
H	-2.558286	0.578922	-2.769360
Si	-1.084610	0.496020	0.423771
H	-2.437987	1.450077	2.324434
H	-0.683965	1.580203	2.643044
H	-1.824418	-3.089664	-0.716663
H	-0.773155	2.072367	-1.543690
C	-2.192107	-2.359526	-1.457772
C	-3.403885	0.342305	-2.097308
C	-1.040064	2.179180	-0.478052
C	-1.473465	0.917815	2.241952
H	-1.373287	-2.149928	-2.169117
Si	1.084610	-0.496020	0.423771
H	-3.019012	-2.831458	-2.020312
H	-3.837133	1.296050	-1.749601
H	-4.170371	-0.187472	-2.691454
H	-0.301389	2.850562	-0.003943
H	-2.028783	2.671279	-0.423721
H	1.824418	3.089664	-0.716663

H	2.028783	-2.671279	-0.423721
H	1.373287	2.149928	-2.169117
H	3.019012	2.831458	-2.020312
H	1.521353	-0.019650	2.881128
H	3.837133	-1.296050	-1.749601
C	1.473465	-0.917815	2.241952
C	1.040064	-2.179180	-0.478052
C	3.403885	-0.342305	-2.097308
C	2.192107	2.359526	-1.457772
H	2.437987	-1.450077	2.324434
H	0.683965	-1.580203	2.643044
H	0.773155	-2.072367	-1.543690
H	0.301389	-2.850562	-0.003943
H	4.170371	0.187472	-2.691454
H	2.558286	-0.578922	-2.769360

MP2/6311G optimized geometry, all-*ortho*-$Si_{10}Me_{22}$**

98
RI-MP2
Energy= -3765.79287878870036
TD B3LYP
Energy= -3773.82982236

H	-0.355649	6.583269	-2.565554
Si	-1.984660	3.951849	-0.144289
C	-3.041203	4.465380	-1.640564
C	-3.121420	2.959702	1.010544
Si	-1.283581	5.890287	1.002795
H	-3.622526	6.515694	1.707104
H	-3.157475	7.620198	-1.627031
H	1.097847	6.953458	-1.629092
Si	-0.959667	7.737673	-0.422635
C	-2.667795	6.359865	2.220758
C	0.287121	5.588740	2.026780
H	-0.002111	10.018409	-0.049793
H	0.883730	8.814184	0.894836
H	0.275702	8.233647	-2.530403
H	-3.874942	5.107542	-1.334191
H	-3.466260	3.585123	-2.135895
H	-2.455404	5.013322	-2.386538
Si	-0.221075	2.603652	-0.945665
H	-2.425709	7.284412	2.757541
H	-2.817824	5.572791	2.967881
C	0.114844	7.335032	-1.923164
C	-2.632413	8.372859	-1.030466
C	-0.114844	9.115004	0.560892
H	-3.989802	3.561872	1.300724
H	-2.608189	2.656557	1.929076
H	-3.493057	2.052826	0.522546
H	-3.283136	8.648117	-0.193763
H	-0.693564	9.388292	1.449833
H	-2.504719	9.263571	-1.656639
H	0.557447	6.490017	2.588628
H	1.142614	5.321028	1.398140
H	0.137762	4.780218	2.749847
H	0.355649	-6.583269	-2.565554
Si	1.984660	-3.951849	-0.144289
C	3.041203	-4.465380	-1.640564
C	3.121420	-2.959702	1.010544
Si	1.283581	-5.890287	1.002795
H	3.622526	-6.515694	1.707104

H	3.157475	-7.620198	-1.627031
H	-1.097847	-6.953458	-1.629092
Si	0.959667	-7.737673	-0.422635
C	2.667795	-6.359865	2.220758
C	-0.287121	-5.588740	2.026780
H	0.002111	-10.018409	-0.049793
H	-0.883730	-8.814184	0.894836
H	-0.275702	-8.233647	-2.530403
H	3.874942	-5.107542	-1.334191
H	3.466260	-3.585123	-2.135895
H	2.455404	-5.013322	-2.386538
Si	0.221075	-2.603652	-0.945665
H	2.425709	-7.284412	2.757541
H	2.817824	-5.572791	2.967881
C	-0.114844	-7.335032	-1.923164
C	2.632413	-8.372859	-1.030466
C	0.114844	-9.115004	0.560892
H	3.989802	-3.561872	1.300724
H	2.608189	-2.656557	1.929076
H	3.493057	-2.052826	0.522546
H	3.283136	-8.648117	-0.193763
H	0.693564	-9.388292	1.449833
H	2.504719	-9.263571	-1.656639
H	-0.557447	-6.490017	2.588628
H	-1.142614	-5.321028	1.398140
H	-0.137762	-4.780218	2.749847
Si	-0.583736	-1.025559	0.613743
C	-1.237964	-3.720465	-1.438386
C	0.809181	-1.743082	-2.534301
H	1.682777	-1.107352	-2.356310
C	-0.535702	-1.733570	2.376306
H	0.021986	-1.114114	-2.962559
C	-2.412947	-0.697327	0.207429
H	0.489056	-1.914042	2.717341
H	-1.079373	-2.681704	2.440693
H	-1.000054	-1.034508	3.080996
Si	0.583736	1.025559	0.613743
H	1.089767	-2.486216	-3.289234
H	-0.924227	-4.487333	-2.155909
H	-2.034536	-3.133177	-1.908962
H	-1.672354	-4.232096	-0.572697
H	-3.001898	-1.616889	0.299191
H	-2.544505	-0.321420	-0.812995
H	-2.843880	0.041435	0.892910
C	1.237964	3.720465	-1.438386

C	-0.809181	1.743082	-2.534301
H	-1.682777	1.107352	-2.356310
C	0.535702	1.733570	2.376306
H	-0.021986	1.114114	-2.962559
C	2.412947	0.697327	0.207429
H	-0.489056	1.914042	2.717341
H	1.079373	2.681704	2.440693
H	1.000054	1.034508	3.080996
H	-1.089767	2.486216	-3.289234
H	0.924227	4.487333	-2.155909
H	2.034536	3.133177	-1.908962
H	1.672354	4.232096	-0.572697
H	3.001898	1.616889	0.299191
H	2.544505	0.321420	-0.812995
H	2.843880	-0.041435	0.892910

MP2/6311G optimized geometry, all-*gauche*-$Si_{10}Me_{22}$**

98
RI-MP2
Energy= -3765.79061176508958
TD B3LYP
Energy= -3773.82327846

Si	-0.840131	3.715402	1.453919
H	0.820979	6.753675	1.148551
H	-2.415413	8.387660	-1.135919
H	-3.890531	6.622692	0.972179
H	-3.379447	3.697111	-2.160500
C	0.937726	3.429526	2.065756
Si	-0.753761	5.370425	-0.218401
C	-1.830453	4.460726	2.897534
H	-1.837132	7.672757	-2.657061
H	-5.116211	6.293002	-0.266242
C	-4.169098	5.946944	0.158247
C	0.491648	4.915792	-1.578264
Si	-2.831898	5.925184	-1.176389
C	-0.139155	6.943169	0.659395
H	-3.570792	7.956615	-2.410031
H	-4.326522	4.948360	0.571292
H	-0.858238	7.272835	1.415007
H	-1.823795	3.776994	3.751800
H	-2.868623	4.643828	2.608892
H	-1.384725	5.407355	3.216773
H	1.615307	3.279229	1.225212
H	0.983807	2.561797	2.728487
H	1.282212	4.305552	2.623974
H	-4.155667	5.002069	-3.067674
H	0.000000	7.750940	-0.065227
Si	-1.903312	1.666923	0.981988
H	0.124621	4.093132	-2.191065
H	1.449198	4.625897	-1.136213
H	0.661849	5.777810	-2.230432
C	-2.642072	7.655440	-1.916373
C	-3.235243	4.701879	-2.558117
H	-2.428490	4.672484	-3.296335
Si	0.840131	-3.715402	1.453919
H	-0.820979	-6.753675	1.148551
H	2.415413	-8.387660	-1.135919
H	3.890531	-6.622692	0.972179
H	3.379447	-3.697111	-2.160500
C	-0.937726	-3.429526	2.065756

Si	0.753761	-5.370425	-0.218401
C	1.830453	-4.460726	2.897534
H	1.837132	-7.672757	-2.657061
H	5.116211	-6.293002	-0.266242
C	4.169098	-5.946944	0.158247
C	-0.491648	-4.915792	-1.578264
Si	2.831898	-5.925184	-1.176389
C	0.139155	-6.943169	0.659395
H	3.570792	-7.956615	-2.410031
H	4.326522	-4.948360	0.571292
H	0.858238	-7.272835	1.415007
H	1.823795	-3.776994	3.751800
H	2.868623	-4.643828	2.608892
H	1.384725	-5.407355	3.216773
H	-1.615307	-3.279229	1.225212
H	-0.983807	-2.561797	2.728487
H	-1.282212	-4.305552	2.623974
H	4.155667	-5.002069	-3.067674
H	0.000000	-7.750940	-0.065227
Si	1.903312	-1.666923	0.981988
H	-0.124621	-4.093132	-2.191065
H	-1.449198	-4.625897	-1.136213
H	-0.661849	-5.777810	-2.230432
C	2.642072	-7.655440	-1.916373
C	3.235243	-4.701879	-2.558117
H	2.428490	-4.672484	-3.296335
Si	1.121522	-0.359895	-0.815182
C	2.241579	1.177068	-0.874232
C	1.401648	-1.296357	-2.446565
H	0.828805	-0.669952	3.011167
C	1.832962	-0.650577	2.587898
H	2.130134	0.385006	2.405460
C	3.742215	-2.005653	0.629915
H	2.518062	-1.077591	3.326861
H	1.141171	-0.658897	-3.296732
H	0.789185	-2.195524	-2.490067
H	2.453908	-1.574996	-2.544215
Si	-1.121522	0.359895	-0.815182
H	1.829532	1.932717	-1.548380
H	3.235607	0.898427	-1.237401
H	2.354806	1.606364	0.121060
H	4.287438	-1.060903	0.543105
H	3.869193	-2.562143	-0.299194
H	4.185589	-2.579505	1.448717
C	-2.241579	-1.177068	-0.874232

C	-1.401648	1.296357	-2.446565
H	-0.828805	0.669952	3.011167
C	-1.832962	0.650577	2.587898
H	-2.130134	-0.385006	2.405460
C	-3.742215	2.005653	0.629915
H	-2.518062	1.077591	3.326861
H	-1.141171	0.658897	-3.296732
H	-0.789185	2.195524	-2.490067
H	-2.453908	1.574996	-2.544215
H	-1.829532	-1.932717	-1.548380
H	-3.235607	-0.898427	-1.237401
H	-2.354806	-1.606364	0.121060
H	-4.287438	1.060903	0.543105
H	-3.869193	2.562143	-0.299194
H	-4.185589	2.579505	1.448717

MP2/6311G optimized geometry, all-*anti*-$Si_{11}Me_{24}$**

107
RI-MP2
Energy= -4134.38812751624846
TD B3LYP
Energy= -4143.21075093

Si	0.000000	9.806731	-0.566054
Si	0.000000	7.837321	0.732361
Si	0.000000	5.875711	-0.579235
Si	0.000000	3.917356	0.741148
Si	0.000000	1.953893	-0.571688
Si	0.000000	0.000000	0.748696
Si	0.000000	-1.953893	-0.571688
Si	0.000000	-3.917356	0.741148
Si	0.000000	-5.875711	-0.579235
Si	0.000000	-7.837321	0.732361
Si	0.000000	-9.806731	-0.566054
C	-1.538280	9.929295	-1.657405
C	0.000000	11.282185	0.619138
C	1.538280	9.929295	-1.657405
C	1.540672	7.893783	1.844490
C	-1.540672	7.893783	1.844490
C	1.540960	5.887450	-1.689053
C	-1.540960	5.887450	-1.689053
C	1.542925	3.933373	1.849307
C	-1.542925	3.933373	1.849307
C	1.541214	1.938071	-1.681453
C	-1.541214	1.938071	-1.681453
C	1.543178	0.000000	1.856855
C	-1.543178	0.000000	1.856855
C	1.541214	-1.938071	-1.681453
C	-1.541214	-1.938071	-1.681453
C	1.542925	-3.933373	1.849307
C	-1.542925	-3.933373	1.849307
C	1.540960	-5.887450	-1.689053
C	-1.540960	-5.887450	-1.689053
C	-1.540672	-7.893783	1.844490
C	1.540672	-7.893783	1.844490
C	1.538280	-9.929295	-1.657405
C	-1.538280	-9.929295	-1.657405
C	0.000000	-11.282185	0.619138
H	0.880151	-11.448236	1.147108
H	-2.462730	5.862923	-1.093938
H	2.462730	5.862923	-1.093938

H	2.456030	9.825265	-1.074356
H	-1.575421	6.788491	-2.309536
H	1.554666	5.021629	-2.359000
H	1.575421	6.788491	-2.309536
H	-1.554666	5.021629	-2.359000
H	1.572395	10.902875	-2.162218
H	-0.880151	11.448236	1.147108
H	0.880151	11.448236	1.147108
H	1.546365	9.156539	-2.434064
H	0.000000	12.227505	0.063979
H	-1.546365	9.156539	-2.434064
H	-2.456030	9.825265	-1.074356
H	-1.572395	10.902875	-2.162218
H	1.590899	8.839462	2.395306
H	-2.461626	7.800814	1.262687
H	-1.530893	7.084491	2.583082
H	-1.590899	8.839462	2.395306
H	2.461626	7.800814	1.262687
H	1.530893	7.084491	2.583082
H	-2.461626	-7.800814	1.262687
H	2.461626	-7.800814	1.262687
H	-1.590899	-8.839462	2.395306
H	1.530893	-7.084491	2.583082
H	1.590899	-8.839462	2.395306
H	-1.530893	-7.084491	2.583082
H	1.572395	-10.902875	-2.162218
H	-2.456030	-9.825265	-1.074356
H	-1.546365	-9.156539	-2.434064
H	-1.572395	-10.902875	-2.162218
H	2.456030	-9.825265	-1.074356
H	1.546365	-9.156539	-2.434064
H	2.462618	3.906870	1.255895
H	-2.462618	3.906870	1.255895
H	-1.554669	3.069946	2.524195
H	-1.572809	4.836807	2.469552
H	1.572809	4.836807	2.469552
H	1.554808	2.801303	-2.354734
H	1.554669	3.069946	2.524195
H	-2.462479	1.964379	-1.086435
H	-1.554808	2.801303	-2.354734
H	-1.575051	1.034241	-2.298453
H	2.462479	1.964379	-1.086435
H	1.575051	1.034241	-2.298453
H	2.462730	-5.862923	-1.093938
H	-2.462730	-5.862923	-1.093938

H	-1.554666	-5.021629	-2.359000
H	-1.575421	-6.788491	-2.309536
H	1.575421	-6.788491	-2.309536
H	1.572809	-4.836807	2.469552
H	1.554666	-5.021629	-2.359000
H	-2.462618	-3.906870	1.255895
H	-1.572809	-4.836807	2.469552
H	-1.554669	-3.069946	2.524195
H	2.462618	-3.906870	1.255895
H	1.554669	-3.069946	2.524195
H	2.462871	0.000000	1.263443
H	-2.462871	0.000000	1.263443
H	-1.554417	-0.851873	2.531742
H	-1.554417	0.851873	2.531742
H	1.554417	0.851873	2.531742
H	1.575051	-1.034241	-2.298453
H	1.554417	-0.851873	2.531742
H	-2.462479	-1.964379	-1.086435
H	-1.575051	-1.034241	-2.298453
H	-1.554808	-2.801303	-2.354734
H	2.462479	-1.964379	-1.086435
H	1.554808	-2.801303	-2.354734
H	-0.880151	-11.448236	1.147108
H	0.000000	-12.227505	0.063979

MP2/6311G optimized geometry, all-*transoid*-$Si_{11}Me_{24}$**

107
RI-MP2
Energy= -4134.37461689119391
TD B3LYP
Energy= -4143.18921759

Si	0.000000	9.651947	-0.180381
Si	-1.079712	7.641750	0.396130
Si	0.078687	5.789104	-0.478597
Si	-0.582450	3.816625	0.620444
Si	0.051354	1.929100	-0.633035
Si	0.000000	0.000000	0.708256
Si	-0.051354	-1.929100	-0.633035
Si	0.582450	-3.816625	0.620444
Si	-0.078687	-5.789104	-0.478597
Si	1.079712	-7.641750	0.396130
Si	0.000000	-9.651947	-0.180381
C	1.568615	9.863016	0.851748
C	-1.146880	11.117520	0.156263
C	0.466169	9.662079	-2.012374
C	-2.842239	7.647585	-0.312883
C	-1.193862	7.536742	2.290335
C	-0.303592	5.667211	-2.335551
C	1.952880	6.010620	-0.261093
C	-2.469164	3.857717	0.839298
C	0.222512	3.707783	2.337757
C	-1.136881	1.680628	-2.094417
C	1.800796	2.210214	-1.318164
C	-1.580527	0.060084	1.775780
C	1.580527	-0.060084	1.775780
C	-1.800796	-2.210214	-1.318164
C	1.136881	-1.680628	-2.094417
C	-0.222512	-3.707783	2.337757
C	2.469164	-3.857717	0.839298
C	-1.952880	-6.010620	-0.261093
C	0.303592	-5.667211	-2.335551
C	1.193862	-7.536742	2.290335
C	2.842239	-7.647585	-0.312883
C	-1.568615	-9.863016	0.851748
C	-0.466169	-9.662079	-2.012374
C	1.146880	-11.117520	0.156263
H	1.509839	-11.115813	1.105379
H	-2.175475	1.599017	-1.756173
H	-2.817736	2.998763	1.423531

H	-1.080175	2.519900	-2.796586
H	-0.897070	0.767672	-2.650749
H	-2.788717	4.765296	1.363408
H	-2.984598	3.834523	-0.126897
H	-0.117930	4.523845	2.985236
H	-0.029485	2.764789	2.834938
H	1.314307	3.767611	2.273030
H	1.856373	3.139961	-1.894715
H	2.540904	2.273931	-0.513201
H	2.100527	1.391406	-1.982094
H	-2.540904	-2.273931	-0.513201
H	-1.612117	-0.777499	2.481536
H	-2.100527	-1.391406	-1.982094
H	-1.856373	-3.139961	-1.894715
H	-1.627140	0.986028	2.359697
H	-2.485108	0.011066	1.160091
H	1.612117	0.777499	2.481536
H	1.627140	-0.986028	2.359697
H	2.485108	-0.011066	1.160091
H	0.897070	-0.767672	-2.650749
H	2.175475	-1.599017	-1.756173
H	1.080175	-2.519900	-2.796586
H	-2.231975	-6.118808	0.721602
H	0.117930	-4.523845	2.985236
H	-2.488343	-5.289047	-0.819805
H	-2.214837	-7.035304	-0.790171
H	0.029485	-2.764789	2.834938
H	-1.314307	-3.767611	2.273030
H	2.817736	-2.998763	1.423531
H	2.788717	-4.765296	1.363408
H	2.984598	-3.834523	-0.126897
H	-0.091894	-4.707575	-2.753734
H	1.457205	-5.516506	-2.483376
H	0.024750	-6.464742	-2.906874
H	-0.648859	12.066184	-0.075848
H	-3.376474	6.724293	-0.064394
H	-1.509839	11.115813	1.105379
H	-2.832460	7.742046	-1.403994
H	1.188512	8.873113	-2.247581
H	0.920770	10.619264	-2.293718
H	-0.409869	9.512472	-2.652698
H	2.488343	5.289047	-0.819805
H	2.231975	6.118808	0.721602
H	2.214837	7.035304	-0.790171
H	-1.457205	5.516506	-2.483376

H	0.091894	4.707575	-2.753734
H	-0.024750	6.464742	-2.906874
H	1.339620	9.890733	1.922394
H	-2.055283	11.062435	-0.452762
H	-0.202219	7.474565	2.751223
H	-1.764404	6.656643	2.606700
H	-1.695731	8.419256	2.703812
H	-3.423255	8.485963	0.087530
H	2.078745	10.799818	0.598819
H	2.275564	9.044091	0.684600
H	-2.275564	-9.044091	0.684600
H	-1.339620	-9.890733	1.922394
H	3.376474	-6.724293	-0.064394
H	2.832460	-7.742046	-1.403994
H	3.423255	-8.485963	0.087530
H	0.202219	-7.474565	2.751223
H	1.764404	-6.656643	2.606700
H	1.695731	-8.419256	2.703812
H	0.409869	-9.512472	-2.652698
H	-1.188512	-8.873113	-2.247581
H	-0.920770	-10.619264	-2.293718
H	-2.078745	-10.799818	0.598819
H	0.648859	-12.066184	-0.075848
H	2.055283	-11.062435	-0.452762

MP2/6311G optimized geometry, all-*deviant*-$Si_{11}Me_{24}$**

107
RI-MP2
Energy= -4134.40459912398001
TD B3LYP
Energy= -4143.22975584

Si	0.000000	9.885023	0.360675
Si	-1.136488	7.878505	-0.227972
Si	0.308623	5.971562	-0.215951
Si	-0.782864	3.918934	0.362665
Si	0.180931	1.994106	-0.692762
Si	0.000000	0.000000	0.626330
Si	-0.180931	-1.994106	-0.692762
Si	0.782864	-3.918934	0.362665
Si	-0.308623	-5.971562	-0.215951
Si	1.136488	-7.878505	-0.227972
Si	0.000000	-9.885023	0.360675
C	0.495516	9.865788	2.194821
C	-1.164143	11.363805	0.083197
C	1.557135	10.165596	-0.692830
C	-1.890585	8.050452	-1.974023
C	-2.584888	7.713232	1.009301
C	1.092239	5.925514	-1.958785
C	1.735492	6.192268	1.035250
C	-2.624230	3.904540	-0.146638
C	-0.721387	3.834464	2.270433
C	-0.699841	1.857463	-2.382742
C	2.048912	2.190953	-1.042955
C	-1.537688	-0.012232	1.760411
C	1.537688	0.012232	1.760411
C	-2.048912	-2.190953	-1.042955
C	0.699841	-1.857463	-2.382742
C	0.721387	-3.834464	2.270433
C	2.624230	-3.904540	-0.146638
C	-1.735492	-6.192268	1.035250
C	-1.092239	-5.925514	-1.958785
C	2.584888	-7.713232	1.009301
C	1.890585	-8.050452	-1.974023
C	-0.495516	-9.865788	2.194821
C	1.164143	-11.363805	0.083197
C	-1.557135	-10.165596	-0.692830
H	-1.317393	-10.207579	-1.752417
H	-1.129137	8.214202	-2.731089
H	2.033358	11.107426	-0.429346

H	-1.458036	11.452508	-0.959434
H	-0.675569	12.293892	0.365561
H	2.293290	9.378686	-0.553350
H	1.317393	10.207579	-1.752417
H	2.336269	7.066381	0.799583
H	2.398919	5.330969	1.017673
H	1.372185	6.304871	2.052453
H	-2.071824	11.279926	0.675187
H	-2.582122	8.888211	-2.014793
H	-2.444857	7.157625	-2.252584
H	1.505131	6.897204	-2.218733
H	0.365718	5.666580	-2.724039
H	1.903486	5.207196	-2.013534
H	0.967686	10.806278	2.470417
H	1.198260	9.068832	2.419418
H	-0.369685	9.735069	2.839657
H	-3.163160	8.633213	1.047524
H	-2.234409	7.506930	2.017151
H	-3.266768	6.917967	0.726383
H	2.582122	-8.888211	-2.014793
H	2.444857	-7.157625	-2.252584
H	1.129137	-8.214202	-2.731089
H	3.163160	-8.633213	1.047524
H	2.234409	-7.506930	2.017151
H	3.266768	-6.917967	0.726383
H	0.289190	3.685655	2.640134
H	2.234572	2.967506	-1.777524
H	-1.337829	3.027698	2.652796
H	-1.094930	4.757985	2.706123
H	2.463146	1.267571	-1.440481
H	2.609182	2.439570	-0.146186
H	-0.226691	1.115922	-3.017849
H	-0.659663	2.806164	-2.912437
H	-1.746678	1.587279	-2.277950
H	-3.070805	2.933699	0.054034
H	-2.756886	4.111817	-1.204672
H	-3.193867	4.641005	0.410615
H	2.457843	-0.141970	1.204202
H	0.226691	-1.115922	-3.017849
H	1.475325	-0.758907	2.521050
H	1.624671	0.965392	2.276333
H	0.659663	-2.806164	-2.912437
H	1.746678	-1.587279	-2.277950
H	-2.234572	-2.967506	-1.777524
H	-2.463146	-1.267571	-1.440481

H	-2.609182	-2.439570	-0.146186
H	-1.624671	-0.965392	2.276333
H	-2.457843	0.141970	1.204202
H	-1.475325	0.758907	2.521050
H	-0.365718	-5.666580	-2.724039
H	3.193867	-4.641005	0.410615
H	-1.903486	-5.207196	-2.013534
H	-1.505131	-6.897204	-2.218733
H	3.070805	-2.933699	0.054034
H	2.756886	-4.111817	-1.204672
H	1.337829	-3.027698	2.652796
H	1.094930	-4.757985	2.706123
H	-0.289190	-3.685655	2.640134
H	-2.398919	-5.330969	1.017673
H	-1.372185	-6.304871	2.052453
H	-2.336269	-7.066381	0.799583
H	-0.967686	-10.806278	2.470417
H	-1.198260	-9.068832	2.419418
H	0.369685	-9.735069	2.839657
H	1.458036	-11.452508	-0.959434
H	0.675569	-12.293892	0.365561
H	2.071824	-11.279926	0.675187
H	-2.033358	-11.107426	-0.429346
H	-2.293290	-9.378686	-0.553350

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{11}Me_{24}$**

107
RI-MP2
Energy= -4134.38458827709746
TD B3LYP
Energy= -4143.20848241

Si	-2.770380	9.303994	0.310741
Si	-3.055447	7.204107	-0.725819
Si	-2.427747	5.352178	0.641948
Si	-0.687626	3.924947	-0.173475
Si	-1.246143	1.619914	-0.514112
Si	0.000000	0.000000	0.738312
Si	1.246143	-1.619914	-0.514112
Si	0.687626	-3.924947	-0.173475
Si	2.427747	-5.352178	0.641948
Si	3.055447	-7.204107	-0.725819
Si	2.770380	-9.303994	0.310741
C	-0.961541	9.630912	0.779431
C	-3.298901	10.639328	-0.932966
C	-3.860708	9.490284	1.851881
C	-4.918184	7.021402	-1.105213
C	-2.175565	7.296121	-2.413995
C	-4.045526	4.435345	1.057647
C	-1.800294	6.000672	2.324543
C	0.000000	4.526614	-1.846745
C	0.765451	4.172002	1.035142
C	-1.120754	1.362071	-2.399011
C	-3.074219	1.242880	-0.125707
C	1.274425	0.790500	1.915554
C	-1.274425	-0.790500	1.915554
C	3.074219	-1.242880	-0.125707
C	1.120754	-1.362071	-2.399011
C	-0.765451	-4.172002	1.035142
C	0.000000	-4.526614	-1.846745
C	1.800294	-6.000672	2.324543
C	4.045526	-4.435345	1.057647
C	2.175565	-7.296121	-2.413995
C	4.918184	-7.021402	-1.105213
C	0.961541	-9.630912	0.779431
C	3.860708	-9.490284	1.851881
C	3.298901	-10.639328	-0.932966
H	3.208463	-11.627340	-0.491398
H	-3.778416	10.496070	2.252942
H	-2.679565	10.619237	-1.823475

H	-4.905320	9.316331	1.614946
H	-0.616952	8.952580	1.551517
H	-3.576767	8.799955	2.637775
H	-0.843144	10.643287	1.153825
H	-1.111205	7.471863	-2.314023
H	-2.311797	6.385718	-2.985943
H	-2.594949	8.112636	-2.993305
H	-5.513516	7.022891	-0.199247
H	-5.257489	7.841752	-1.729653
H	-5.124093	6.097974	-1.636147
H	-4.535291	4.030282	0.181319
H	-3.864540	3.620699	1.749204
H	-4.736676	5.122407	1.535336
H	-0.888320	6.577414	2.230984
H	-2.549980	6.627253	2.794907
H	-1.599836	5.173786	2.997983
H	-3.208463	11.627340	-0.491398
H	-0.307464	9.520543	-0.079623
H	-4.331300	10.510242	-1.240902
H	4.905320	-9.316331	1.614946
H	3.576767	-8.799955	2.637775
H	3.778416	-10.496070	2.252942
H	0.307464	-9.520543	-0.079623
H	0.843144	-10.643287	1.153825
H	0.616952	-8.952580	1.551517
H	1.111205	-7.471863	-2.314023
H	2.311797	-6.385718	-2.985943
H	2.594949	-8.112636	-2.993305
H	5.513516	-7.022891	-0.199247
H	5.257489	-7.841752	-1.729653
H	5.124093	-6.097974	-1.636147
H	-3.319846	1.365981	0.920925
H	0.851270	3.918043	-2.134754
H	-3.727557	1.887207	-0.702645
H	-3.301311	0.217918	-0.401437
H	0.530688	3.868201	2.047019
H	-0.123023	1.527565	-2.784025
H	1.634865	3.613026	0.709308
H	1.042776	5.220974	1.059868
H	-0.728709	4.475883	-2.645372
H	0.343931	5.551781	-1.769994
H	-1.423884	0.357612	-2.670233
H	-1.789300	2.051893	-2.904345
H	0.728709	-4.475883	-2.645372
H	1.599836	-5.173786	2.997983

H	-0.343931	-5.551781	-1.769994
H	-0.851270	-3.918043	-2.134754
H	4.535291	-4.030282	0.181319
H	-0.530688	-3.868201	2.047019
H	3.864540	-3.620699	1.749204
H	4.736676	-5.122407	1.535336
H	0.888320	-6.577414	2.230984
H	2.549980	-6.627253	2.794907
H	-1.634865	-3.613026	0.709308
H	-1.042776	-5.220974	1.059868
H	-2.070766	-1.305711	1.394702
H	3.301311	-0.217918	-0.401437
H	-0.794022	-1.498452	2.580742
H	-1.726124	-0.019394	2.531702
H	0.123023	-1.527565	-2.784025
H	2.070766	1.305711	1.394702
H	1.423884	-0.357612	-2.670233
H	1.789300	-2.051893	-2.904345
H	3.319846	-1.365981	0.920925
H	3.727557	-1.887207	-0.702645
H	0.794022	1.498452	2.580742
H	1.726124	0.019394	2.531702
H	4.331300	-10.510242	-1.240902
H	2.679565	-10.619237	-1.823475

MP2/6311G optimized geometry, all-*ortho*-$Si_{11}Me_{24}$**

107
RI-MP2
Energy= -4134.41090174080909
TD B3LYP
Energy= -4143.22247295

Si	-0.851267	8.569873	-0.854999
Si	0.000000	6.944260	0.621212
Si	-1.370465	5.034081	0.820892
Si	-0.936351	3.353164	-0.777744
Si	0.758105	1.832639	-0.155955
Si	0.000000	0.000000	1.123151
Si	-0.758105	-1.832639	-0.155955
Si	0.936351	-3.353164	-0.777744
Si	1.370465	-5.034081	0.820892
Si	0.000000	-6.944260	0.621212
Si	0.851267	-8.569873	-0.854999
C	-1.543582	7.825385	-2.444335
C	0.560113	9.718777	-1.331783
C	-2.180485	9.604404	-0.039016
C	0.138130	7.730569	2.347881
C	1.761549	6.483387	0.080335
C	-1.182225	4.352706	2.584425
C	-3.190048	5.554292	0.628432
C	-2.560372	2.417794	-1.096247
C	-0.430785	4.146133	-2.429890
C	2.096746	2.731450	0.849439
C	1.595196	1.210585	-1.744290
C	1.423202	-0.547305	2.258179
C	-1.423202	0.547305	2.258179
C	-2.096746	-2.731450	0.849439
C	-1.595196	-1.210585	-1.744290
C	2.560372	-2.417794	-1.096247
C	0.430785	-4.146133	-2.429890
C	3.190048	-5.554292	0.628432
C	1.182225	-4.352706	2.584425
C	-0.138130	-7.730569	2.347881
C	-1.761549	-6.483387	0.080335
C	1.543582	-7.825385	-2.444335
C	-0.560113	-9.718777	-1.331783
C	2.180485	-9.604404	-0.039016
H	2.981094	-9.007001	0.346815
H	-2.392459	7.172090	-2.247525
H	-2.981094	9.007001	0.346815

H	-0.789403	7.240130	-2.968888
H	0.206234	10.528056	-1.978942
H	1.336907	9.184782	-1.869962
H	-1.884756	8.613547	-3.124620
H	-1.760428	10.164068	0.771009
H	1.020581	10.168178	-0.453004
H	-2.614012	10.304223	-0.752242
H	-0.844057	7.993831	2.754855
H	0.741676	8.644809	2.318823
H	0.614761	7.041651	3.053730
H	2.401807	7.371980	0.065937
H	1.781813	6.045326	-0.922502
H	2.211694	5.761208	0.768246
H	-3.452187	6.346419	1.339135
H	-3.858004	4.706328	0.816916
H	-3.405018	5.926349	-0.379085
H	-1.479213	5.109339	3.319357
H	-0.148571	4.066436	2.804676
H	-1.811918	3.470960	2.741121
H	-2.954440	1.958978	-0.183283
H	-2.421816	1.621831	-1.835865
H	-3.327519	3.098872	-1.481092
H	-0.323016	3.381094	-3.206844
H	0.524394	4.676391	-2.354228
H	-1.183770	4.863878	-2.772848
H	1.714553	3.091440	1.809888
H	2.490668	3.595095	0.303133
H	2.936285	2.059562	1.059377
H	2.396649	0.499015	-1.518266
H	2.038263	2.045607	-2.297859
H	0.885885	0.711759	-2.412275
H	2.310620	-0.842906	1.688744
H	1.128959	-1.398261	2.881714
H	1.717267	0.268769	2.927321
H	-1.128959	1.398261	2.881714
H	-1.717267	-0.268769	2.927321
H	-2.310620	0.842906	1.688744
H	-0.885885	-0.711759	-2.412275
H	-2.396649	-0.499015	-1.518266
H	-2.038263	-2.045607	-2.297859
H	-2.936285	-2.059562	1.059377
H	-1.714553	-3.091440	1.809888
H	-2.490668	-3.595095	0.303133
H	-0.524394	-4.676391	-2.354228
H	1.183770	-4.863878	-2.772848

H	0.323016	-3.381094	-3.206844
H	3.327519	-3.098872	-1.481092
H	2.954440	-1.958978	-0.183283
H	2.421816	-1.621831	-1.835865
H	0.148571	-4.066436	2.804676
H	1.811918	-3.470960	2.741121
H	1.479213	-5.109339	3.319357
H	3.452187	-6.346419	1.339135
H	3.858004	-4.706328	0.816916
H	3.405018	-5.926349	-0.379085
H	-0.741676	-8.644809	2.318823
H	-0.614761	-7.041651	3.053730
H	0.844057	-7.993831	2.754855
H	-2.401807	-7.371980	0.065937
H	-1.781813	-6.045326	-0.922502
H	-2.211694	-5.761208	0.768246
H	-1.020581	-10.168178	-0.453004
H	-0.206234	-10.528056	-1.978942
H	-1.336907	-9.184782	-1.869962
H	1.884756	-8.613547	-3.124620
H	2.392459	-7.172090	-2.247525
H	0.789403	-7.240130	-2.968888
H	1.760428	-10.164068	0.771009
H	2.614012	-10.304223	-0.752242

MP2/6311G optimized geometry, all-*gauche*-$Si_{11}Me_{24}$**

107
RI-MP2
Energy= -4134.40416219716462
TD B3LYP
Energy= -4143.21287740

Si	1.792169	7.287185	0.591798
Si	-0.172392	6.054330	0.975329
Si	-0.878419	4.605892	-0.741983
Si	0.613216	2.967738	-1.541771
Si	1.486676	1.382623	-0.034220
Si	0.000000	0.000000	1.160429
Si	-1.486676	-1.382623	-0.034220
Si	-0.613216	-2.967738	-1.541771
Si	0.878419	-4.605892	-0.741983
Si	0.172392	-6.054330	0.975329
Si	-1.792169	-7.287185	0.591798
C	3.317390	6.218922	0.872080
C	1.798221	8.676078	1.866531
C	1.816932	8.066780	-1.108006
C	-1.571438	7.325472	1.160472
C	0.000000	5.129618	2.624632
C	-1.315732	5.678654	-2.250177
C	-2.491238	3.792608	-0.147746
C	2.112133	3.832314	-2.331582
C	-0.296891	2.073436	-2.952489
C	2.688271	0.308449	-1.044019
C	2.535352	2.282390	1.272617
C	1.083481	-1.075367	2.295383
C	-1.083481	1.075367	2.295383
C	-2.535352	-2.282390	1.272617
C	-2.688271	-0.308449	-1.044019
C	-2.112133	-3.832314	-2.331582
C	0.296891	-2.073436	-2.952489
C	2.491238	-3.792608	-0.147746
C	1.315732	-5.678654	-2.250177
C	1.571438	-7.325472	1.160472
C	0.000000	-5.129618	2.624632
C	-1.798221	-8.676078	1.866531
C	-3.317390	-6.218922	0.872080
C	-1.816932	-8.066780	-1.108006
H	-2.603538	-8.774664	-1.120673
H	0.945769	9.336387	1.714745
H	0.886678	8.557579	-1.325065

H	3.399676	5.467430	0.107213
H	1.748535	8.269732	2.872181
H	2.603538	8.774664	-1.120673
H	2.716161	9.262298	1.782846
H	2.009130	7.334702	-1.847505
H	4.220247	6.826443	0.851965
H	3.270143	5.731761	1.834824
H	-2.512918	6.819674	1.381211
H	-1.694747	7.903878	0.243941
H	-1.354446	8.014137	1.982139
H	0.911678	4.544275	2.648837
H	-0.850473	4.470382	2.781923
H	0.036707	5.841536	3.451083
H	-1.761969	5.060366	-3.034203
H	-0.427553	6.164010	-2.657958
H	-2.040554	6.448969	-1.971403
H	-2.368964	3.383322	0.854651
H	-2.796446	2.996200	-0.830616
H	-3.291407	4.538255	-0.112528
H	-0.384361	2.738183	-3.816719
H	-1.302649	1.791659	-2.643362
H	0.252014	1.181995	-3.262720
H	1.780490	4.542928	-3.092322
H	2.758746	3.095233	-2.815942
H	2.697902	4.362927	-1.582277
H	1.907278	2.812681	1.974665
H	3.210630	2.985963	0.799307
H	3.133278	1.566687	1.831532
H	3.591503	0.881521	-1.275236
H	2.233574	0.005205	-1.986782
H	2.982651	-0.579434	-0.479632
H	1.923178	-1.494095	1.740849
H	0.499009	-1.887702	2.734767
H	1.487364	-0.464915	3.108958
H	-1.487364	0.464915	3.108958
H	-1.923178	1.494095	1.740849
H	-0.499009	1.887702	2.734767
H	-3.591503	-0.881521	-1.275236
H	-2.233574	-0.005205	-1.986782
H	-2.982651	0.579434	-0.479632
H	-3.210630	-2.985963	0.799307
H	-3.133278	-1.566687	1.831532
H	-1.907278	-2.812681	1.974665
H	-2.758746	-3.095233	-2.815942
H	-2.697902	-4.362927	-1.582277

H	-1.780490	-4.542928	-3.092322
H	-0.252014	-1.181995	-3.262720
H	0.384361	-2.738183	-3.816719
H	1.302649	-1.791659	-2.643362
H	2.368964	-3.383322	0.854651
H	2.796446	-2.996200	-0.830616
H	3.291407	-4.538255	-0.112528
H	1.761969	-5.060366	-3.034203
H	0.427553	-6.164010	-2.657958
H	2.040554	-6.448969	-1.971403
H	2.512918	-6.819674	1.381211
H	1.694747	-7.903878	0.243941
H	1.354446	-8.014137	1.982139
H	-0.911678	-4.544275	2.648837
H	0.850473	-4.470382	2.781923
H	-0.036707	-5.841536	3.451083
H	-1.748535	-8.269732	2.872181
H	-0.945769	-9.336387	1.714745
H	-2.716161	-9.262298	1.782846
H	-3.399676	-5.467430	0.107213
H	-3.270143	-5.731761	1.834824
H	-4.220247	-6.826443	0.851965
H	-0.886678	-8.557579	-1.325065
H	-2.009130	-7.334702	-1.847505

MP2/6311G optimized geometry, all-*anti*-$Si_{12}Me_{26}$**

116
RI-MP2
Energy= -4503.03269992843525
TD B3LYP
Energy= -4512.62976416

H	1.174314	6.851547	-2.462000
H	1.174314	6.851547	2.462000
C	1.729472	10.918936	-1.537000
H	1.144546	10.813527	2.457000
Si	0.637559	10.794173	0.000000
C	-0.550470	12.267343	0.000000
C	1.729472	10.918936	1.537000
H	2.387666	7.779395	-1.574000
H	2.438901	6.012430	1.556000
H	2.387666	7.779395	1.574000
H	2.438901	6.012430	-1.556000
H	2.230792	11.893286	1.574000
H	-1.197468	12.263891	-0.884000
H	-1.197468	12.263891	0.884000
H	2.506012	10.147478	1.548000
H	0.002868	13.213730	0.000000
H	2.506012	10.147478	-1.548000
H	1.144546	10.813527	-2.457000
H	2.230792	11.893286	-1.574000
Si	-0.658306	4.902293	0.000000
H	-2.322762	9.821104	1.590000
H	-1.186037	8.784898	-2.462000
Si	0.658306	6.863186	0.000000
H	-2.505535	8.065976	-1.532000
H	-2.322762	9.821104	-1.590000
H	-1.186037	8.784898	2.462000
H	-2.505535	8.065976	1.532000
C	1.767297	6.876961	1.542000
C	1.767297	6.876961	-1.542000
Si	-0.657063	8.822268	0.000000
C	-1.770101	8.876490	1.540000
C	-1.770101	8.876490	-1.540000
H	-1.174314	-6.851547	-2.462000
H	-1.174314	-6.851547	2.462000
C	-1.729472	-10.918936	-1.537000
H	-1.144546	-10.813527	2.457000
Si	-0.637559	-10.794173	0.000000
C	0.550470	-12.267343	0.000000

C	-1.729472	-10.918936	1.537000
H	-2.387666	-7.779395	-1.574000
H	-2.438901	-6.012430	1.556000
H	-2.387666	-7.779395	1.574000
H	-2.438901	-6.012430	-1.556000
H	-2.230792	-11.893286	1.574000
H	1.197468	-12.263891	-0.884000
H	1.197468	-12.263891	0.884000
H	-2.506012	-10.147478	1.548000
H	-0.002868	-13.213730	0.000000
H	-2.506012	-10.147478	-1.548000
H	-1.144546	-10.813527	-2.457000
H	-2.230792	-11.893286	-1.574000
Si	0.658306	-4.902293	0.000000
H	2.322762	-9.821104	1.590000
H	1.186037	-8.784898	-2.462000
Si	-0.658306	-6.863186	0.000000
H	2.505535	-8.065976	-1.532000
H	2.322762	-9.821104	-1.590000
H	1.186037	-8.784898	2.462000
H	2.505535	-8.065976	1.532000
C	-1.767297	-6.876961	1.542000
C	-1.767297	-6.876961	-1.542000
Si	0.657063	-8.822268	0.000000
C	1.770101	-8.876490	1.540000
C	1.770101	-8.876490	-1.540000
H	-1.174314	4.890658	2.462000
C	1.767297	2.927575	-1.542000
H	-1.174314	4.890658	-2.462000
C	1.767297	2.927575	1.542000
Si	0.658306	2.941360	0.000000
H	-2.438909	4.051553	-1.556000
H	-2.387658	5.818517	-1.574000
H	-2.387658	5.818517	1.574000
H	2.438909	3.792100	1.556000
H	-2.438909	4.051553	1.556000
H	1.174314	2.952995	-2.462000
H	2.438909	3.792100	-1.556000
C	-1.767297	4.916078	-1.542000
H	2.387658	2.025135	-1.574000
H	1.174314	2.952995	2.462000
C	-1.767297	4.916078	1.542000
H	2.387658	2.025135	1.574000
Si	-0.658306	0.980466	0.000000
H	1.174314	-4.890658	2.462000

C	-1.767297	-2.927575	-1.542000
H	1.174314	-4.890658	-2.462000
C	-1.767297	-2.927575	1.542000
Si	-0.658306	-2.941360	0.000000
H	2.438909	-4.051553	-1.556000
H	2.387658	-5.818517	-1.574000
H	2.387658	-5.818517	1.574000
H	-2.438909	-3.792100	1.556000
H	2.438909	-4.051553	1.556000
H	-1.174314	-2.952995	-2.462000
H	-2.438909	-3.792100	-1.556000
C	1.767297	-4.916078	-1.542000
H	-2.387658	-2.025135	-1.574000
H	-1.174314	-2.952995	2.462000
C	1.767297	-4.916078	1.542000
H	-2.387658	-2.025135	1.574000
Si	0.658306	-0.980466	0.000000
H	-1.174314	0.968832	2.462000
C	1.767297	-0.994251	-1.542000
H	-1.174314	0.968832	-2.462000
C	1.767297	-0.994251	1.542000
H	-2.438909	0.129727	-1.556000
H	-2.387658	1.896691	-1.574000
H	-2.387658	1.896691	1.574000
H	2.438909	-0.129727	1.556000
H	-2.438909	0.129727	1.556000
H	1.174314	-0.968832	-2.462000
H	2.438909	-0.129727	-1.556000
C	-1.767297	0.994251	-1.542000
H	2.387658	-1.896691	-1.574000
H	1.174314	-0.968832	2.462000
C	-1.767297	0.994251	1.542000
H	2.387658	-1.896691	1.574000

MP2/6311G optimized geometry, all-*transoid*-$Si_{12}Me_{26}$**

116
RI-MP2
Energy= -4503.04362392871462
TD B3LYP
Energy= -4512.63059139

Si	-0.620166	2.890760	-0.162017
Si	0.589353	4.808323	0.467015
C	2.376541	4.633826	-0.153053
C	0.620166	4.975291	2.359222
H	-1.963363	2.719395	1.958270
C	-2.195597	2.732937	0.887929
H	1.155283	4.137938	2.820875
C	-1.124219	3.057659	-1.986037
H	-2.877324	3.571159	0.705537
H	-2.737551	1.809625	0.654940
H	1.122064	5.898841	2.668509
Si	0.682301	0.958322	0.161917
Si	-0.411967	6.738977	-0.430538
H	-0.392691	4.993455	2.775796
H	2.997882	5.466653	0.195404
H	2.833514	3.706689	0.209607
H	2.421439	4.620205	-1.247395
H	-1.679858	3.985380	-2.160760
H	-0.248911	3.065831	-2.644485
H	-1.766010	2.224953	-2.295541
Si	-0.682301	-0.958322	0.161917
C	1.976333	0.786746	-1.218306
C	1.589249	1.120103	1.823407
H	-0.886113	-1.136434	2.663096
C	-1.589249	-1.120103	1.823407
H	2.277063	0.281845	1.981111
C	-1.976333	-0.786746	-1.218306
H	-2.277063	-0.281845	1.981111
H	-2.178022	-2.043138	1.866494
H	2.178022	2.043138	1.866494
Si	0.620166	-2.890760	-0.162017
H	0.886113	1.136434	2.663096
H	2.689007	1.619032	-1.196308
H	2.548883	-0.141076	-1.112174
H	1.507396	0.776167	-2.208140
H	-2.548883	0.141076	-1.112174
H	-1.507396	-0.776167	-2.208140
H	-2.689007	-1.619032	-1.196308

Si	-0.589353	-4.808323	0.467015
C	1.124219	-3.057659	-1.986037
C	2.195597	-2.732937	0.887929
H	0.392691	-4.993455	2.775796
C	-0.620166	-4.975291	2.359222
H	2.877324	-3.571159	0.705537
C	-2.376541	-4.633826	-0.153053
H	-1.155283	-4.137938	2.820875
H	-1.122064	-5.898841	2.668509
H	2.737551	-1.809625	0.654940
Si	0.411967	-6.738977	-0.430538
H	1.963363	-2.719395	1.958270
H	1.766010	-2.224953	-2.295541
H	1.679858	-3.985380	-2.160760
H	0.248911	-3.065831	-2.644485
H	-2.833514	-3.706689	0.209607
H	-2.421439	-4.620205	-1.247395
H	-2.997882	-5.466653	0.195404
C	-1.847509	10.587148	-1.226369
C	0.169443	12.133622	0.495126
H	0.000728	13.048017	-0.085632
H	-0.330648	7.902610	2.978807
C	-2.299186	6.655659	-0.228708
Si	0.368110	8.659721	0.683715
C	-0.006339	6.831927	-2.284129
C	1.114428	10.693919	-2.047639
H	1.184901	12.184263	0.902576
H	-1.595771	8.890267	2.236986
C	2.240014	8.549943	0.993543
Si	-0.071211	10.596223	-0.579610
C	-0.512399	8.789356	2.362146
H	-2.020342	9.752790	-1.914515
H	-2.069409	11.513308	-1.769515
H	-2.573670	10.501360	-0.410789
H	-0.310484	5.916484	-2.803157
H	1.067286	6.968296	-2.453000
H	-0.527475	7.670270	-2.760245
H	-2.583596	6.514747	0.819624
H	-2.721415	5.823584	-0.803172
H	-2.777492	7.576430	-0.580715
H	2.157294	10.729849	-1.715027
H	-0.527524	12.144113	1.339679
H	2.796288	8.417832	0.059334
H	2.486272	7.708287	1.650164
H	2.613383	9.461544	1.474424

H	-0.160487	9.662356	2.923231
H	0.926045	11.595802	-2.641712
H	1.007380	9.830254	-2.711699
C	1.847509	-10.587148	-1.226369
C	-0.169443	-12.133622	0.495126
H	-0.000728	-13.048017	-0.085632
H	0.330648	-7.902610	2.978807
C	2.299186	-6.655659	-0.228708
Si	-0.368110	-8.659721	0.683715
C	0.006339	-6.831927	-2.284129
C	-1.114428	-10.693919	-2.047639
H	-1.184901	-12.184263	0.902576
H	1.595771	-8.890267	2.236986
C	-2.240014	-8.549943	0.993543
Si	0.071211	-10.596223	-0.579610
C	0.512399	-8.789356	2.362146
H	2.020342	-9.752790	-1.914515
H	2.069409	-11.513308	-1.769515
H	2.573670	-10.501360	-0.410789
H	0.310484	-5.916484	-2.803157
H	-1.067286	-6.968296	-2.453000
H	0.527475	-7.670270	-2.760245
H	2.583596	-6.514747	0.819624
H	2.721415	-5.823584	-0.803172
H	2.777492	-7.576430	-0.580715
H	-2.157294	-10.729849	-1.715027
H	0.527524	-12.144113	1.339679
H	-2.796288	-8.417832	0.059334
H	-2.486272	-7.708287	1.650164
H	-2.613383	-9.461544	1.474424
H	0.160487	-9.662356	2.923231
H	-0.926045	-11.595802	-2.641712
H	-1.007380	-9.830254	-2.711699

MP2/6311G optimized geometry, all-*deviant*-$Si_{12}Me_{26}$**

116
RI-MP2
Energy= -4503.02747953813832
TD B3LYP
Energy= -4512.61761897

H	-3.104686	8.936318	0.118314
Si	-0.276198	6.791041	-0.629052
C	1.233930	6.978077	-1.778058
C	-1.824987	6.630477	-1.732157
Si	-0.651002	8.720141	0.684264
C	2.026632	10.606720	-0.516369
H	-0.208007	11.667679	-2.704811
H	-1.499423	12.282755	0.546371
Si	0.132134	10.637265	-0.441222
C	-2.516273	8.848761	1.049122
C	0.279100	8.675939	2.350843
H	-0.003526	13.103040	0.010472
H	-0.241701	9.883921	-2.817260
H	-1.665584	10.767154	-2.196094
H	1.098266	7.824378	-2.476096
H	1.370565	6.060183	-2.380490
H	2.162908	7.150290	-1.205673
H	-0.018550	12.182350	1.542648
H	-2.729214	9.735421	1.674670
H	-2.871043	7.954551	1.594799
C	-0.398579	12.195533	0.505018
C	-0.560460	10.746227	-2.204170
Si	0.103845	4.862913	0.682527
H	-2.034199	7.588861	-2.243441
H	-2.716996	6.361810	-1.137696
H	-1.682884	5.857342	-2.507447
H	2.406434	11.522043	-1.008209
H	2.394424	9.735000	-1.085456
H	2.462277	10.562090	0.498337
H	0.184211	9.647050	2.871825
H	1.355651	8.473428	2.204351
H	-0.127393	7.895638	3.017878
H	3.104686	-8.936318	0.118314
Si	0.276198	-6.791041	-0.629052
C	-1.233930	-6.978077	-1.778058
C	1.824987	-6.630477	-1.732157
Si	0.651002	-8.720141	0.684264
C	-2.026632	-10.606720	-0.516369

H	0.208007	-11.667679	-2.704811
H	1.499423	-12.282755	0.546371
Si	-0.132134	-10.637265	-0.441222
C	2.516273	-8.848761	1.049122
C	-0.279100	-8.675939	2.350843
H	0.003526	-13.103040	0.010472
H	0.241701	-9.883921	-2.817260
H	1.665584	-10.767154	-2.196094
H	-1.098266	-7.824378	-2.476096
H	-1.370565	-6.060183	-2.380490
H	-2.162908	-7.150290	-1.205673
H	0.018550	-12.182350	1.542648
H	2.729214	-9.735421	1.674670
H	2.871043	-7.954551	1.594799
C	0.398579	-12.195533	0.505018
C	0.560460	-10.746227	-2.204170
Si	-0.103845	-4.862913	0.682527
H	2.034199	-7.588861	-2.243441
H	2.716996	-6.361810	-1.137696
H	1.682884	-5.857342	-2.507447
H	-2.406434	-11.522043	-1.008209
H	-2.394424	-9.735000	-1.085456
H	-2.462277	-10.562090	0.498337
H	-0.184211	-9.647050	2.871825
H	-1.355651	-8.473428	2.204351
H	0.127393	-7.895638	3.017878
Si	-0.657310	2.888647	-0.368695
C	-2.493156	2.688431	0.105930
C	-0.560460	2.990467	-2.271752
H	2.549172	4.631363	0.076544
C	1.984814	4.841110	1.003233
H	-1.267717	3.740736	-2.666580
C	-0.769269	4.953530	2.375201
H	2.252261	4.073047	1.749931
H	2.320498	5.821540	1.390213
H	-0.816048	2.013278	-2.722812
H	0.455565	3.264152	-2.609445
Si	0.633112	0.997350	0.214537
H	-2.942423	1.818464	-0.407103
H	-3.063876	3.588762	-0.190388
H	-2.619984	2.548672	1.194353
H	-0.560642	4.038550	2.961211
H	-1.864668	5.043841	2.264619
H	-0.410167	5.819849	2.960371
Si	-0.633112	-0.997350	0.214537

C	-1.407089	-1.154605	1.950024
C	-2.059385	-0.957151	-1.052547
H	1.692058	0.709711	-2.065014
C	2.059385	0.957151	-1.052547
H	-2.820966	-0.209080	-0.770784
C	1.407089	1.154605	1.950024
H	2.820966	0.209080	-0.770784
H	2.556344	1.944106	-1.103860
H	-2.556344	-1.944106	-1.103860
H	-1.692058	-0.709711	-2.065014
Si	0.657310	-2.888647	-0.368695
H	-2.075095	-2.033421	2.007788
H	-2.008725	-0.255524	2.181998
H	-0.634768	-1.257987	2.733040
H	2.008725	0.255524	2.181998
H	0.634768	1.257987	2.733040
H	2.075095	2.033421	2.007788
C	2.493156	-2.688431	0.105930
C	0.560460	-2.990467	-2.271752
H	-2.549172	-4.631363	0.076544
C	-1.984814	-4.841110	1.003233
H	1.267717	-3.740736	-2.666580
C	0.769269	-4.953530	2.375201
H	-2.252261	-4.073047	1.749931
H	-2.320498	-5.821540	1.390213
H	0.816048	-2.013278	-2.722812
H	-0.455565	-3.264152	-2.609445
H	2.942423	-1.818464	-0.407103
H	3.063876	-3.588762	-0.190388
H	2.619984	-2.548672	1.194353
H	0.560642	-4.038550	2.961211
H	1.864668	-5.043841	2.264619
H	0.410167	-5.819849	2.960371

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{12}Me_{26}$**

116
RI-MP2
Energy= -4503.00160065751516
TD B3LYP
Energy= -4512.59531971

Si	-10.404046	-1.823792	0.712867
Si	-8.491610	-2.029281	-0.654158
Si	-6.811127	-0.417587	-0.156707
H	-12.194154	-0.114475	1.082544
H	-11.210204	-4.184109	0.349341
C	-11.636246	-3.175472	0.200885
C	-7.919674	-3.844547	-0.543684
C	-9.033418	-1.746248	-2.463422
C	-6.706890	0.725223	-1.679212
C	-7.383081	0.711576	1.273733
H	-11.520496	0.030034	-0.566370
H	-9.312884	-1.289812	2.922654
H	-10.618067	0.688665	0.829737
H	-10.907074	-2.064545	3.154831
H	-7.637196	-4.129946	0.484489
H	-7.051938	-4.035017	-1.200223
H	-8.743687	-4.506713	-0.868741
H	-9.438654	-0.729931	-2.614383
H	-9.817441	-2.473301	-2.746096
H	-8.182991	-1.878345	-3.157714
H	-6.388908	0.186764	-2.588326
H	-5.995175	1.551467	-1.502597
H	-7.700861	1.168472	-1.875407
H	-7.529547	0.150258	2.212724
H	-8.337167	1.206029	1.016032
H	-6.633004	1.501380	1.464186
H	-12.559520	-3.104295	0.806500
H	-9.490320	-3.056112	2.704736
H	-11.920315	-3.078073	-0.862641
C	-11.258619	-0.145228	0.492912
C	-9.984534	-2.080519	2.544517
Si	-4.693033	-1.278254	0.523426
Si	10.404046	1.823792	0.712867
Si	8.491610	2.029281	-0.654158
Si	6.811127	0.417587	-0.156707
H	12.194154	0.114475	1.082544
H	11.210204	4.184109	0.349341
C	11.636246	3.175472	0.200885

C	7.919674	3.844547	-0.543684
C	9.033418	1.746248	-2.463422
C	6.706890	-0.725223	-1.679212
C	7.383081	-0.711576	1.273733
H	11.520496	-0.030034	-0.566370
H	9.312884	1.289812	2.922654
H	10.618067	-0.688665	0.829737
H	10.907074	2.064545	3.154831
H	7.637196	4.129946	0.484489
H	7.051938	4.035017	-1.200223
H	8.743687	4.506713	-0.868741
H	9.438654	0.729931	-2.614383
H	9.817441	2.473301	-2.746096
H	8.182991	1.878345	-3.157714
H	6.388908	-0.186764	-2.588326
H	5.995175	-1.551467	-1.502597
H	7.700861	-1.168472	-1.875407
H	7.529547	-0.150258	2.212724
H	8.337167	-1.206029	1.016032
H	6.633004	-1.501380	1.464186
H	12.559520	3.104295	0.806500
H	9.490320	3.056112	2.704736
H	11.920315	3.078073	-0.862641
C	11.258619	0.145228	0.492912
C	9.984534	2.080519	2.544517
Si	4.693033	1.278254	0.523426
H	-3.710275	1.318523	-2.121563
H	-3.772351	-3.588981	0.916297
Si	-2.828700	-0.693671	-0.844778
H	-4.075915	-0.206214	-2.980477
H	-2.421614	0.469478	-3.022508
H	-4.446013	0.324068	2.479908
H	-1.802522	-3.014551	-0.729651
C	-4.477205	-0.771062	2.348549
C	-4.731507	-3.187849	0.539745
C	-2.164593	-2.347768	-1.531236
C	-3.312103	0.323285	-2.383291
H	-3.546196	-1.193943	2.766644
Si	-1.074378	0.517762	0.225007
H	-5.324770	-1.161758	2.941789
H	-4.902699	-3.608333	-0.466297
H	-5.535021	-3.551069	1.205787
H	-1.329164	-2.166337	-2.231463
H	-2.959514	-2.882141	-2.083707
H	3.710275	-1.318523	-2.121563

H	3.772351	3.588981	0.916297
Si	2.828700	0.693671	-0.844778
H	4.075915	0.206214	-2.980477
H	2.421614	-0.469478	-3.022508
H	4.446013	-0.324068	2.479908
H	1.802522	3.014551	-0.729651
C	4.477205	0.771062	2.348549
C	4.731507	3.187849	0.539745
C	2.164593	2.347768	-1.531236
C	3.312103	-0.323285	-2.383291
H	3.546196	1.193943	2.766644
Si	1.074378	-0.517762	0.225007
H	5.324770	1.161758	2.941789
H	4.902699	3.608333	-0.466297
H	5.535021	3.551069	1.205787
H	1.329164	2.166337	-2.231463
H	2.959514	2.882141	-2.083707
H	-0.846145	2.227102	-1.641097
H	0.718238	-1.422751	2.547854
H	-0.332495	2.908754	-0.070186
H	-2.071506	2.715581	-0.435649
H	0.846145	-2.227102	-1.641097
H	-1.577462	-0.140971	2.626206
C	1.074378	-2.254341	-0.561881
C	1.498715	-0.806096	2.064871
C	-1.498715	0.806096	2.064871
C	-1.074378	2.254341	-0.561881
H	0.332495	-2.908754	-0.070186
H	2.071506	-2.715581	-0.435649
H	1.577462	0.140971	2.626206
H	2.460195	-1.342679	2.158725
H	-2.460195	1.342679	2.158725
H	-0.718238	1.422751	2.547854

MP2/6311G optimized geometry, all-*ortho*-$Si_{12}Me_{26}$**

116
RI-MP2
Energy= -4503.03466841638237
TD B3LYP
Energy= -4512.62065371

H	-2.734323	8.221861	-0.375455
Si	0.158543	6.027237	1.126386
C	-1.050237	6.779539	2.388025
C	1.614283	5.319673	2.121569
Si	0.985076	7.744294	-0.264087
H	2.218881	8.891266	1.612086
H	-1.180430	9.875234	1.782798
H	-2.214547	8.240073	-2.065470
Si	-0.574812	9.473652	-0.618596
C	2.484055	8.515647	0.617990
C	1.596726	7.081451	-1.935346
H	-0.579634	11.468251	-2.128310
H	0.176652	10.086542	-2.932118
H	-2.949118	9.680681	-1.349773
H	-0.579896	7.595899	2.948107
H	-1.374070	6.024416	3.113146
H	-1.948214	7.180616	1.905683
Si	-0.985076	4.311086	-0.021235
H	2.891474	9.356058	0.044188
H	3.286787	7.780917	0.744403
C	-2.272756	8.840691	-1.152102
C	-0.776900	10.482524	0.966439
C	0.088236	10.612426	-1.975671
H	2.079861	6.105248	2.727382
H	2.389657	4.901006	1.471556
H	1.285578	4.526233	2.800602
H	0.180058	10.896784	1.300953
H	1.077705	11.007801	-1.721803
H	-1.462801	11.322615	0.806581
H	2.022548	7.892549	-2.536882
H	0.789008	6.625970	-2.517459
H	2.377213	6.325828	-1.798547
H	2.734323	-8.221861	-0.375455
Si	-0.158543	-6.027237	1.126386
C	1.050237	-6.779539	2.388025
C	-1.614283	-5.319673	2.121569
Si	-0.985076	-7.744294	-0.264087
H	-2.218881	-8.891266	1.612086

H	1.180430	-9.875234	1.782798
H	2.214547	-8.240073	-2.065470
Si	0.574812	-9.473652	-0.618596
C	-2.484055	-8.515647	0.617990
C	-1.596726	-7.081451	-1.935346
H	0.579634	-11.468251	-2.128310
H	-0.176652	-10.086542	-2.932118
H	2.949118	-9.680681	-1.349773
H	0.579896	-7.595899	2.948107
H	1.374070	-6.024416	3.113146
H	1.948214	-7.180616	1.905683
Si	0.985076	-4.311086	-0.021235
H	-2.891474	-9.356058	0.044188
H	-3.286787	-7.780917	0.744403
C	2.272756	-8.840691	-1.152102
C	0.776900	-10.482524	0.966439
C	-0.088236	-10.612426	-1.975671
H	-2.079861	-6.105248	2.727382
H	-2.389657	-4.901006	1.471556
H	-1.285578	-4.526233	2.800602
H	-0.180058	-10.896784	1.300953
H	-1.077705	-11.007801	-1.721803
H	1.462801	-11.322615	0.806581
H	-2.022548	-7.892549	-2.536882
H	-0.789008	-6.625970	-2.517459
H	-2.377213	-6.325828	-1.798547
Si	0.406128	2.581280	-0.822596
C	-0.427937	1.840010	-2.363275
C	2.082846	3.271928	-1.389903
H	2.659892	3.683292	-0.555157
C	-2.325625	3.618623	1.133597
H	1.956714	4.067825	-2.131065
C	-1.888688	5.061740	-1.517511
H	-1.899485	3.201841	2.052129
H	-2.902790	2.826524	0.645600
Si	0.811429	0.856765	0.736843
H	-3.025368	4.410490	1.423777
H	2.685478	2.480585	-1.849805
H	0.166693	1.017898	-2.777888
H	-0.537423	2.597472	-3.147584
H	-1.426574	1.449175	-2.139999
H	-2.511384	4.308231	-2.012841
H	-1.189128	5.454190	-2.263485
H	-2.545251	5.884186	-1.211138
Si	-0.811429	-0.856765	0.736843

C	0.860160	1.602276	2.486322
C	2.541436	0.147720	0.398391
H	2.623550	-0.267204	-0.611608
C	-2.541436	-0.147720	0.398391
H	2.792018	-0.648849	1.106465
C	-0.860160	-1.602276	2.486322
H	-2.623550	0.267204	-0.611608
H	-2.792018	0.648849	1.106465
H	-3.300846	-0.931708	0.496162
Si	-0.406128	-2.581280	-0.822596
H	3.300846	0.931708	0.496162
H	1.590444	2.417233	2.548676
H	1.147006	0.843856	3.223476
H	-0.113504	2.003762	2.787429
H	-1.147006	-0.843856	3.223476
H	0.113504	-2.003762	2.787429
H	-1.590444	-2.417233	2.548676
C	1.888688	-5.061740	-1.517511
C	2.325625	-3.618623	1.133597
H	1.899485	-3.201841	2.052129
C	-2.082846	-3.271928	-1.389903
H	2.902790	-2.826524	0.645600
C	0.427937	-1.840010	-2.363275
H	-2.659892	-3.683292	-0.555157
H	-1.956714	-4.067825	-2.131065
H	-2.685478	-2.480585	-1.849805
H	3.025368	-4.410490	1.423777
H	2.545251	-5.884186	-1.211138
H	2.511384	-4.308231	-2.012841
H	1.189128	-5.454190	-2.263485
H	0.537423	-2.597472	-3.147584
H	1.426574	-1.449175	-2.139999
H	-0.166693	-1.017898	-2.777888

MP2/6311G optimized geometry, all-*gauche*-$Si_{12}Me_{26}$**

116
RI-MP2
Energy= -4503.03212819524924
TD B3LYP
Energy= -4512.61244135

Si	4.925123	-2.274581	-0.351860
H	7.077170	-2.739366	-3.039204
H	10.236298	-0.718532	-0.969368
H	8.825161	-2.305315	1.315237
H	6.577910	1.372912	1.524668
C	3.857862	-2.889147	-1.801034
Si	6.697084	-1.019420	-1.261773
C	5.711997	-3.799741	0.469715
H	9.651284	0.893827	-1.435675
H	9.236270	-0.966768	2.403329
C	8.476148	-1.348898	1.715463
C	6.062401	0.343650	-2.422022
Si	8.185358	-0.109213	0.319592
C	7.712662	-2.257395	-2.290272
H	10.536134	0.674285	0.086163
H	7.559573	-1.521271	2.283536
H	8.147493	-3.030466	-1.649967
H	4.932650	-4.479147	0.827901
H	6.336133	-3.510420	1.319073
H	6.331560	-4.343027	-0.249774
H	3.604600	-2.065916	-2.469075
H	2.939348	-3.354157	-1.434304
H	4.412278	-3.634856	-2.379127
H	8.226703	2.004228	1.628250
H	8.523494	-1.740322	-2.811938
Si	3.579430	-1.306807	1.322017
H	5.602025	1.156924	-1.862069
H	5.327446	-0.063248	-3.122407
H	6.894709	0.756874	-2.999911
C	9.810392	0.215733	-0.592038
C	7.499378	1.528842	0.963442
H	7.292440	2.213643	0.135867
Si	-4.925123	2.274581	-0.351860
H	-7.077170	2.739366	-3.039204
H	-10.236298	0.718532	-0.969368
H	-8.825161	2.305315	1.315237
H	-6.577910	-1.372912	1.524668
C	-3.857862	2.889147	-1.801034

Si	-6.697084	1.019420	-1.261773
C	-5.711997	3.799741	0.469715
H	-9.651284	-0.893827	-1.435675
H	-9.236270	0.966768	2.403329
C	-8.476148	1.348898	1.715463
C	-6.062401	-0.343650	-2.422022
Si	-8.185358	0.109213	0.319592
C	-7.712662	2.257395	-2.290272
H	-10.536134	-0.674285	0.08616
H	-7.559573	1.521271	2.283536
H	-8.147493	3.030466	-1.649967
H	-4.932650	4.479147	0.827901
H	-6.336133	3.510420	1.319073
H	-6.331560	4.343027	-0.249774
H	-3.604600	2.065916	-2.469075
H	-2.939348	3.354157	-1.434304
H	-4.412278	3.634856	-2.379127
H	-8.226703	-2.004228	1.628250
H	-8.523494	1.740322	-2.811938
Si	-3.579430	1.306807	1.322017
H	-5.602025	-1.156924	-1.862069
H	-5.327446	0.063248	-3.122407
H	-6.894709	-0.756874	-2.999911
C	-9.810392	-0.215733	-0.592038
C	-7.499378	-1.528842	0.963442
H	-7.292440	-2.213643	0.135867
Si	2.432386	0.696237	0.851440
C	4.668617	-0.949468	2.840652
C	2.338125	-2.648740	1.846633
H	4.262902	1.880245	-0.385001
C	3.694251	2.080317	0.521494
H	4.383605	2.170446	1.364619
C	1.532979	1.169354	2.460009
H	3.179439	3.038425	0.402107
Si	0.910248	0.747514	-0.945726
H	2.859915	-3.447765	2.382374
H	1.855980	-3.088300	0.973898
H	1.577695	-2.232846	2.511837
H	5.207436	-1.852431	3.141729
H	4.045947	-0.629435	3.681611
H	5.392120	-0.161456	2.629610
H	2.258860	1.520215	3.200174
H	1.017381	0.305997	2.879983
H	0.814270	1.972165	2.279994
Si	-0.910248	-0.747514	-0.945726

C	-1.858755	-0.412390	-2.560739
C	-0.274518	-2.537159	-1.045163
H	0.000000	2.903793	-0.056029
C	0.274518	2.537159	-1.045163
H	-0.589514	2.606020	-1.710543
C	1.858755	0.412390	-2.560739
H	1.061568	3.187968	-1.438654
H	-1.061568	-3.187968	-1.438654
H	0.000000	-2.903793	-0.056029
H	0.589514	-2.606020	-1.710543
Si	-2.432386	-0.696237	0.851440
H	-2.828847	-0.916538	-2.553385
H	-1.283398	-0.786727	-3.413096
H	-2.010916	0.657757	-2.700897
H	1.283398	0.786727	-3.413096
H	2.010916	-0.657757	-2.700897
H	2.828847	0.916538	-2.553385
C	-1.532979	-1.169354	2.460009
C	-3.694251	-2.080317	0.521494
H	-1.855980	3.088300	0.973898
C	-2.338125	2.648740	1.846633
H	-1.577695	2.232846	2.511837
C	-4.668617	0.949468	2.840652
H	-2.859915	3.447765	2.382374
H	-3.179439	-3.038425	0.402107
H	-4.262902	-1.880245	-0.385001
H	-4.383605	-2.170446	1.364619
H	-0.814270	-1.972165	2.279994
H	-2.258860	-1.520215	3.200174
H	-1.017381	-0.305997	2.879983
H	-4.045947	0.629435	3.681611
H	-5.392120	0.161456	2.629610
H	-5.207436	1.852431	3.141729

MP2/6311G optimized geometry, all-*anti*-$Si_{13}Me_{28}$**

125
RI-MP2
Energy= -4871.65274187883460
TD B3LYP
Energy= -4882.02524246

Si	0.000000	-11.770351	0.576969
Si	0.000000	-9.800067	-0.720120
Si	0.000000	-7.839342	0.592798
Si	0.000000	-5.880097	-0.726267
Si	0.000000	-3.917519	0.587892
Si	0.000000	-1.958274	-0.731173
Si	0.000000	0.000000	0.582968
Si	0.000000	1.958274	-0.731173
Si	0.000000	3.917519	0.587892
Si	0.000000	5.880097	-0.726267
Si	0.000000	7.839342	0.592798
Si	0.000000	9.800067	-0.720120
Si	0.000000	11.770351	0.576969
C	-1.537000	-11.893748	1.669037
C	0.000000	-13.245006	-0.609217
C	1.537000	-11.893748	1.669037
C	1.540000	-9.855681	-1.833089
C	-1.540000	-9.855681	-1.833089
C	1.542000	-7.851730	1.701805
C	-1.542000	-7.851730	1.701805
C	1.542000	-5.895269	-1.835238
C	-1.542000	-5.895269	-1.835238
C	1.542000	-3.902347	1.696864
C	-1.542000	-3.902347	1.696864
C	1.542000	-1.973446	-1.840144
C	-1.542000	-1.973446	-1.840144
C	1.542000	0.000000	1.691975
C	-1.542000	0.000000	1.691975
C	1.542000	1.973446	-1.840144
C	-1.542000	1.973446	-1.840144
C	1.542000	3.902347	1.696864
C	-1.542000	3.902347	1.696864
C	1.542000	5.895269	-1.835238
C	-1.542000	5.895269	-1.835238
C	1.542000	7.851730	1.701805
C	-1.542000	7.851730	1.701805
C	1.540000	9.855681	-1.833089
C	-1.540000	9.855681	-1.833089

C	1.537000	11.893748	1.669037
C	-1.537000	11.893748	1.669037
C	0.000000	13.245006	-0.609217
H	-0.884000	13.242364	-1.256218
H	-2.462000	-7.827057	1.108791
H	2.462000	-7.827057	1.108791
H	2.457000	-11.789071	1.083979
H	-1.574000	-8.753387	2.323303
H	1.556000	-6.986359	2.372327
H	1.574000	-8.753387	2.323303
H	-1.556000	-6.986359	2.372327
H	1.574000	-12.867471	2.171575
H	-0.884000	-13.242364	-1.256218
H	0.884000	-13.242364	-1.256218
H	1.548000	-11.121319	2.444611
H	0.000000	-14.190700	-0.054695
H	-1.548000	-11.121319	2.444611
H	-2.457000	-11.789071	1.083979
H	-1.574000	-12.867471	2.171575
H	1.590000	-10.800987	-2.384567
H	-2.462000	-9.763359	-1.249140
H	-1.532000	-9.046088	-2.569536
H	-1.590000	-10.800987	-2.384567
H	2.462000	-9.763359	-1.249140
H	1.532000	-9.046088	-2.569536
H	1.574000	-6.798484	-2.454471
H	2.462000	-5.869107	-1.242289
H	-1.556000	-1.109762	-2.512837
H	1.556000	-4.766031	2.369557
H	1.556000	-5.031585	-2.507931
H	-1.574000	-2.999131	2.316097
H	-2.462000	-3.928508	1.103915
H	-2.462000	-5.869107	-1.242289
H	-1.574000	-2.876661	-2.459377
H	1.574000	-2.876661	-2.459377
H	1.556000	-1.109762	-2.512837
H	2.462000	-3.928508	1.103915
H	-1.556000	-5.031585	-2.507931
H	-1.574000	-6.798484	-2.454471
H	2.462000	-1.947285	-1.247195
H	-2.462000	-1.947285	-1.247195
H	-1.556000	-4.766031	2.369557
H	1.574000	-2.999131	2.316097
H	-2.462000	0.000000	1.098961
H	2.462000	0.000000	1.098961

H	1.556000	0.857261	2.362497
H	1.556000	-0.857261	2.362497
H	-1.556000	-0.857261	2.362497
H	-1.556000	1.109762	-2.512837
H	-1.556000	0.857261	2.362497
H	2.462000	1.947285	-1.247195
H	1.556000	1.109762	-2.512837
H	1.574000	2.876661	-2.459377
H	-2.462000	1.947285	-1.247195
H	-1.574000	2.876661	-2.459377
H	-2.462000	9.763359	-1.249140
H	2.462000	9.763359	-1.249140
H	-1.590000	10.800987	-2.384567
H	1.532000	9.046088	-2.569536
H	1.590000	10.800987	-2.384567
H	-1.532000	9.046088	-2.569536
H	1.574000	12.867471	2.171575
H	-2.457000	11.789071	1.083979
H	-1.548000	11.121319	2.444611
H	-1.574000	12.867471	2.171575
H	2.457000	11.789071	1.083979
H	1.548000	11.121319	2.444611
H	1.574000	8.753387	2.323303
H	2.462000	7.827057	1.108791
H	-1.574000	2.999131	2.316097
H	1.574000	6.798484	-2.454471
H	1.556000	6.986359	2.372327
H	-1.556000	5.031585	-2.507931
H	-2.462000	5.869107	-1.242289
H	-2.462000	7.827057	1.108791
H	-1.556000	4.766031	2.369557
H	1.556000	4.766031	2.369557
H	1.574000	2.999131	2.316097
H	2.462000	5.869107	-1.242289
H	-1.556000	6.986359	2.372327
H	-1.574000	8.753387	2.323303
H	2.462000	3.928508	1.103915
H	-2.462000	3.928508	1.103915
H	-1.574000	6.798484	-2.454471
H	1.556000	5.031585	-2.507931
H	0.000000	14.190700	-0.054695
H	0.884000	13.242364	-1.256218

MP2/6311G optimized geometry, all-*transoid*-$Si_{13}Me_{28}$**

125
RI-MP2
Energy= -4871.66514174859640
TD B3LYP
Energy= -4882.02680954

Si	0.000000	11.573017	0.067718
Si	-1.196829	9.570318	-0.241627
Si	0.111821	7.718367	0.387003
Si	-0.787500	5.737951	-0.510121
Si	0.092158	3.861297	0.603435
Si	-0.274944	1.911924	-0.661803
Si	0.000000	0.000000	0.681547
Si	0.274944	-1.911924	-0.661803
Si	-0.092158	-3.861297	0.603435
Si	0.787500	-5.737951	-0.510121
Si	-0.111821	-7.718367	0.387003
Si	1.196829	-9.570318	-0.241627
Si	0.000000	-11.573017	0.067718
C	1.276832	11.762218	-1.318721
C	-1.174610	13.053581	0.028296
C	0.907003	11.566654	1.730986
C	-2.775146	9.588308	0.815030
C	-1.697233	9.444368	-2.070092
C	0.160097	7.591759	2.281635
C	1.886664	7.953351	-0.247486
C	-2.677172	5.793529	-0.323470
C	-0.366986	5.596670	-2.357279
C	-0.738589	3.647037	2.298436
C	1.952578	4.135609	0.873024
C	-2.035772	1.975019	-1.371937
C	0.955653	1.817899	-2.105955
C	-1.521000	-0.254516	1.790988
C	1.521000	0.254516	1.790988
C	-0.955653	-1.817899	-2.105955
C	2.035772	-1.975019	-1.371937
C	-1.952578	-4.135609	0.873024
C	0.738589	-3.647037	2.298436
C	0.366986	-5.596670	-2.357279
C	2.677172	-5.793529	-0.323470
C	-1.886664	-7.953351	-0.247486
C	-0.160097	-7.591759	2.281635
C	1.697233	-9.444368	-2.070092
C	2.775146	-9.588308	0.815030

C	-1.276832	-11.762218	-1.318721
C	-0.907003	-11.566654	1.730986
C	1.174610	-13.053581	0.028296
H	0.614072	-13.990406	0.032037
H	-1.796138	13.040088	-0.865832
H	-0.614072	13.990406	0.032037
H	-1.828872	13.049088	0.897523
H	1.657925	10.771211	1.773838
H	1.425843	12.517798	1.897868
H	0.794933	11.802539	-2.300821
H	1.854397	12.685327	-1.195723
H	1.983966	10.926973	-1.330137
H	0.215496	11.416701	2.566511
H	-2.330911	8.568604	-2.248420
H	-3.334615	8.652712	0.711875
H	-2.543681	9.720621	1.876896
H	-0.820948	9.359560	-2.721345
H	-2.260877	10.328897	-2.387431
H	-3.439093	10.406166	0.515216
H	2.335368	8.861835	0.161994
H	-0.840552	7.455299	2.700617
H	0.772265	6.746461	2.605862
H	0.584286	8.495206	2.727149
H	1.916359	8.032655	-1.337512
H	2.523702	7.113378	0.040168
H	-3.146977	4.929374	-0.806517
H	-3.095061	6.696184	-0.782546
H	-2.975700	5.788898	0.730335
H	-0.832064	6.406289	-2.930879
H	-0.724343	4.648792	-2.774420
H	0.713935	5.646942	-2.526791
H	-1.827174	3.570768	2.204006
H	-0.519947	4.496537	2.955240
H	-0.385097	2.740622	2.802085
H	2.142427	5.073711	1.406056
H	2.492816	4.179899	-0.078780
H	2.389159	3.324322	1.466371
H	0.838999	0.884062	-2.666775
H	1.991443	1.865538	-1.753082
H	-2.222004	1.127407	-2.041026
H	-2.198911	2.892534	-1.947893
H	0.804478	2.645830	-2.807724
H	-2.789190	1.943852	-0.577559
H	2.440924	0.320949	1.200161
H	-1.435563	-1.176565	2.376422

H	-1.637779	0.575421	2.496973
H	-2.440924	-0.320949	1.200161
H	1.637779	-0.575421	2.496973
H	1.435563	1.176565	2.376422
H	2.198911	-2.892534	-1.947893
H	2.789190	-1.943852	-0.577559
H	-0.804478	-2.645830	-2.807724
H	-0.838999	-0.884062	-2.666775
H	2.222004	-1.127407	-2.041026
H	-1.991443	-1.865538	-1.753082
H	1.827174	-3.570768	2.204006
H	-2.142427	-5.073711	1.406056
H	-2.389159	-3.324322	1.466371
H	-2.492816	-4.179899	-0.078780
H	0.519947	-4.496537	2.955240
H	0.385097	-2.740622	2.802085
H	-0.713935	-5.646942	-2.526791
H	0.832064	-6.406289	-2.930879
H	0.724343	-4.648792	-2.774420
H	3.095061	-6.696184	-0.782546
H	2.975700	-5.788898	0.730335
H	3.146977	-4.929374	-0.806517
H	-2.523702	-7.113378	0.040168
H	-2.335368	-8.861835	0.161994
H	-1.916359	-8.032655	-1.337512
H	-0.584286	-8.495206	2.727149
H	-0.772265	-6.746461	2.605862
H	0.840552	-7.455299	2.700617
H	3.439093	-10.406166	0.515216
H	0.820948	-9.359560	-2.721345
H	2.330911	-8.568604	-2.248420
H	2.260877	-10.328897	-2.387431
H	2.543681	-9.720621	1.876896
H	3.334615	-8.652712	0.711875
H	1.796138	-13.040088	-0.865832
H	-1.657925	-10.771211	1.773838
H	-1.983966	-10.926973	-1.330137
H	-0.794933	-11.802539	-2.300821
H	-0.215496	-11.416701	2.566511
H	-1.425843	-12.517798	1.897868
H	-1.854397	-12.685327	-1.195723
H	1.828872	-13.049088	0.897523

MP2/6311G optimized geometry, all-*deviant*-$Si_{13}Me_{28}$**

125
RI-MP2
Energy= -4871.64664385665583
TD B3LYP
Energy= -4882.01210809

Si	-0.529929	11.615893	-0.560823
Si	0.376240	9.717594	0.508970
Si	-0.804668	7.755080	-0.071732
Si	0.573544	5.836195	-0.074494
Si	-0.604733	3.874121	0.511062
Si	0.266042	1.946663	-0.541609
Si	0.000000	0.000000	0.770220
Si	-0.266042	-1.946663	-0.541609
Si	0.604733	-3.874121	0.511062
Si	-0.573544	-5.836195	-0.074494
Si	0.804668	-7.755080	-0.071732
Si	-0.376240	-9.717594	0.508970
Si	0.529929	-11.615893	-0.560823
C	0.080665	11.674874	-2.338060
C	-2.413066	11.610802	-0.577199
C	0.000000	13.190246	0.343471
C	2.208037	9.658740	-0.022262
C	0.322173	9.881593	2.406030
C	-1.589745	7.867672	-1.805145
C	-2.223305	7.633277	1.197929
C	1.328550	5.737137	-1.823205
C	2.013210	5.972420	1.169240
C	-0.523809	3.763643	2.412257
C	-2.443524	3.954974	0.015212
C	2.135581	2.090163	-0.891159
C	-0.627572	1.819690	-2.221836
C	1.536090	-0.085952	1.895586
C	-1.536090	0.085952	1.895586
C	-2.135581	-2.090163	-0.891159
C	0.627572	-1.819690	-2.221836
C	0.523809	-3.763643	2.412257
C	2.443524	-3.954974	0.015212
C	-2.013210	-5.972420	1.169240
C	-1.328550	-5.737137	-1.823205
C	2.223305	-7.633277	1.197929
C	1.589745	-7.867672	-1.805145
C	-0.322173	-9.881593	2.406030
C	-2.208037	-9.658740	-0.022262

C	-0.080665	-11.674874	-2.338060
C	0.000000	-13.190246	0.343471
C	2.413066	-11.610802	-0.577199
H	1.172423	11.718306	-2.375694
H	-0.357599	14.071437	-0.184829
H	-0.394407	13.199814	1.333538
H	1.653929	0.860405	2.451511
H	-1.653929	-0.860405	2.451511
H	1.444715	-0.902170	2.632080
H	2.457295	-0.253893	1.312780
H	-2.457295	0.253893	1.312780
H	-1.444715	0.902170	2.632080
H	-2.707365	-2.283306	0.032803
H	-2.515698	-1.152249	-1.334674
H	0.198326	-1.012249	-2.838955
H	1.705143	-1.617965	-2.094073
H	-2.344413	-2.908369	-1.600994
H	0.524506	-2.765851	-2.783190
H	2.707365	2.283306	0.032803
H	2.344413	2.908369	-1.600994
H	2.515698	1.152249	-1.334674
H	-1.705143	1.617965	-2.094073
H	-0.198326	1.012249	-2.838955
H	-0.524506	2.765851	-2.783190
H	-0.507840	-3.597543	2.765624
H	2.564623	-4.136389	-1.065867
H	2.945310	-3.002159	0.257747
H	1.150951	-2.938320	2.789918
H	0.890467	-4.701938	2.863923
H	2.966932	-4.760834	0.557217
H	-2.966932	4.760834	0.557217
H	-1.150951	2.938320	2.789918
H	-0.890467	4.701938	2.863923
H	0.507840	3.597543	2.765624
H	-2.945310	3.002159	0.257747
H	-2.564623	4.136389	-1.065867
H	-2.083809	-4.935120	-1.883958
H	-2.603001	-5.038013	1.176773
H	-1.825349	-6.690089	-2.080670
H	-0.556987	-5.540575	-2.587717
H	-1.647354	-6.149682	2.195229
H	-2.692872	-6.798644	0.899984
H	0.556987	5.540575	-2.587717
H	1.647354	6.149682	2.195229
H	2.603001	5.038013	1.176773

H	2.083809	4.935120	-1.883958
H	1.825349	6.690089	-2.080670
H	2.692872	6.798644	0.899984
H	2.775810	-8.590136	1.250328
H	1.840412	-7.407325	2.209345
H	2.941104	-6.842796	0.917743
H	2.306992	-8.706767	-1.861450
H	2.139141	-6.935597	-2.035896
H	0.826438	-8.015104	-2.589523
H	-2.941104	6.842796	0.917743
H	-2.139141	6.935597	-2.035896
H	-2.775810	8.590136	1.250328
H	-1.840412	7.407325	2.209345
H	-0.826438	8.015104	-2.589523
H	-2.306992	8.706767	-1.861450
H	-0.897554	-10.764315	2.739039
H	-2.692402	-10.637185	0.155148
H	-2.307603	-9.421260	-1.096715
H	-0.764024	-8.987962	2.883929
H	-2.766163	-8.897315	0.550025
H	0.713176	-9.987032	2.774868
H	2.692402	10.637185	0.155148
H	2.307603	9.421260	-1.096715
H	2.766163	8.897315	0.550025
H	0.897554	10.764315	2.739039
H	0.764024	8.987962	2.883929
H	-0.713176	9.987032	2.774868
H	0.238813	-10.786574	-2.889296
H	-1.172423	-11.718306	-2.375694
H	0.317636	-12.565135	-2.859699
H	2.814727	-12.544623	-1.006944
H	0.394407	-13.199814	1.333538
H	0.357599	-14.071437	-0.184829
H	2.794994	-10.784891	-1.165834
H	2.806894	-11.513783	0.428577
H	-1.070122	-13.229864	0.401904
H	1.070122	13.229864	0.401904
H	-0.317636	12.565135	-2.859699
H	-2.814727	12.544623	-1.006944
H	-2.806894	11.513783	0.428577
H	-0.238813	10.786574	-2.889296
H	-2.794994	10.784891	-1.165834

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{13}Me_{28}$**

125
RI-MP2
Energy=-4871.61890283404227
TD B3LYP
Energy= -4881.98777663

Si	-3.721842	10.983413	0.312825
Si	-4.325707	8.695735	0.187310
Si	-2.667796	7.280925	-0.776497
Si	-1.844154	5.524502	0.611342
Si	-2.161120	3.303597	-0.198985
Si	-0.183527	2.017092	-0.550440
Si	0.000000	0.000000	0.709388
Si	0.183527	-2.017092	-0.550440
Si	2.161120	-3.303597	-0.198985
Si	1.844154	-5.524502	0.611342
Si	2.667796	-7.280925	-0.776497
Si	4.325707	-8.695735	0.187310
Si	3.721842	-10.983413	0.312825
C	-2.169343	11.319333	1.352767
C	-5.155724	11.938381	1.123750
C	-3.455155	11.664038	-1.437502
C	-5.881844	8.522443	-0.904557
C	-4.864856	8.179406	1.941391
C	-3.395697	6.660287	-2.425670
C	-1.130969	8.304198	-1.265656
C	0.000000	5.914621	0.901427
C	-2.638262	5.561969	2.344915
C	-3.094012	3.284516	-1.861514
C	-3.339859	2.462731	1.041219
C	1.390801	3.018991	-0.156861
C	-0.106232	1.687743	-2.427327
C	1.493073	0.247217	1.868770
C	-1.493073	-0.247217	1.868770
C	0.106232	-1.687743	-2.427327
C	-1.390801	-3.018991	-0.156861
C	3.094012	-3.284516	-1.861514
C	3.339859	-2.462731	1.041219
C	0.000000	-5.914621	0.901427
C	2.638262	-5.561969	2.344915
C	1.130969	-8.304198	-1.265656
C	3.395697	-6.660287	-2.425670
C	4.864856	-8.179406	1.941391
C	5.881844	-8.522443	-0.904557

C	5.155724	-11.938381	1.123750
C	2.169343	-11.319333	1.352767
C	3.455155	-11.664038	-1.437502
H	3.243318	-12.747705	-1.389176
H	-4.921525	13.018340	1.166932
H	-2.289663	10.941459	2.383179
H	-6.095427	11.816124	0.556429
H	-3.243318	12.747705	-1.389176
H	-5.334314	11.589179	2.156996
H	-4.360611	11.508555	-2.049474
H	-1.272912	10.846667	0.916440
H	-2.603318	11.158912	-1.926140
H	-1.987212	12.406496	1.411136
H	-6.706907	9.132389	-0.494907
H	-6.221479	7.471699	-0.936551
H	-4.045388	8.270734	2.674919
H	-5.222498	7.134560	1.956728
H	-5.695870	8.828128	2.274816
H	-5.695633	8.849157	-1.942482
H	-1.412861	9.111735	-1.965359
H	-0.642048	8.763862	-0.389375
H	-4.305163	6.052297	-2.281694
H	-0.386252	7.662321	-1.771676
H	-2.657739	6.049653	-2.976066
H	-3.661290	7.526438	-3.059844
H	0.581742	5.902411	-0.035378
H	-2.477903	6.544010	2.825129
H	-3.723562	5.369131	2.311289
H	0.448561	5.180543	1.594719
H	0.105584	6.917334	1.353598
H	-2.176073	4.790444	2.986949
H	-2.519001	3.767790	-2.668352
H	-3.595276	1.441975	0.704387
H	-4.278531	3.040183	1.118120
H	-4.063400	3.806494	-1.769627
H	-3.296687	2.242233	-2.166682
H	-2.902362	2.391802	2.050531
H	-0.109964	2.645928	-2.977666
H	1.420379	3.947772	-0.754527
H	0.821962	1.148984	-2.689846
H	2.287585	2.424443	-0.408563
H	1.454970	3.294218	0.909126
H	-0.962450	1.089996	-2.781956
H	2.435394	0.381875	1.312841
H	-2.435394	-0.381875	1.312841

H	1.611380	-0.621344	2.541249
H	1.337781	1.143699	2.495429
H	-1.611380	0.621344	2.541249
H	-1.337781	-1.143699	2.495429
H	-0.821962	-1.148984	-2.689846
H	0.109964	-2.645928	-2.977666
H	-1.420379	-3.947772	-0.754527
H	-2.287585	-2.424443	-0.408563
H	0.962450	-1.089996	-2.781956
H	-1.454970	-3.294218	0.909126
H	3.595276	-1.441975	0.704387
H	4.278531	-3.040183	1.118120
H	2.519001	-3.767790	-2.668352
H	2.902362	-2.391802	2.050531
H	4.063400	-3.806494	-1.769627
H	3.296687	-2.242233	-2.166682
H	3.723562	-5.369131	2.311289
H	-0.448561	-5.180543	1.594719
H	-0.105584	-6.917334	1.353598
H	2.477903	-6.544010	2.825129
H	2.176073	-4.790444	2.986949
H	-0.581742	-5.902411	-0.035378
H	4.305163	-6.052297	-2.281694
H	1.412861	-9.111735	-1.965359
H	0.642048	-8.763862	-0.389375
H	2.657739	-6.049653	-2.976066
H	3.661290	-7.526438	-3.059844
H	0.386252	-7.662321	-1.771676
H	6.706907	-9.132389	-0.494907
H	5.695633	-8.849157	-1.942482
H	4.045388	-8.270734	2.674919
H	6.221479	-7.471699	-0.936551
H	5.222498	-7.134560	1.956728
H	5.695870	-8.828128	2.274816
H	2.603318	-11.158912	-1.926140
H	4.921525	-13.018340	1.166932
H	5.334314	-11.589179	2.156996
H	1.272912	-10.846667	0.916440
H	2.289663	-10.941459	2.383179
H	1.987212	-12.406496	1.411136
H	6.095427	-11.816124	0.556429
H	4.360611	-11.508555	-2.049474

MP2/6311G optimized geometry, all-*ortho*-$Si_{13}Me_{28}$**

125
RI-MP2
Energy= -4871.65260230461536
TD B3LYP
Energy= -4882.01318813

Si	-0.048224	10.391190	0.078522
Si	1.032872	8.553166	-0.925787
Si	1.482608	6.784588	0.569835
Si	-0.264350	5.210614	0.769560
Si	-0.199038	3.475772	-0.829034
Si	1.131784	1.628581	-0.207255
Si	0.000000	0.000000	1.071817
Si	-1.131784	-1.628581	-0.207255
Si	0.199038	-3.475772	-0.829034
Si	0.264350	-5.210614	0.769560
Si	-1.482608	-6.784588	0.569835
Si	-1.032872	-8.553166	-0.925787
Si	0.048224	-10.391190	0.078522
C	-1.427739	9.874322	1.255652
C	-0.823523	11.428837	-1.286089
C	1.164782	11.476574	1.002891
C	2.700094	9.154948	-1.615986
C	0.000000	7.965767	-2.407776
C	3.092630	5.939236	0.019415
C	1.808386	7.504360	2.300152
C	-0.192159	4.478683	2.522392
C	-1.944865	6.085210	0.612482
C	0.463600	4.142439	-2.480170
C	-1.984281	2.908820	-1.147388
C	1.855295	0.861921	-1.787893
C	2.606184	2.246396	0.823564
C	1.273613	-0.838488	2.206851
C	-1.273613	0.838488	2.206851
C	-1.855295	-0.861921	-1.787893
C	-2.606184	-2.246396	0.823564
C	-0.463600	-4.142439	-2.480170
C	1.984281	-2.908820	-1.147388
C	1.944865	-6.085210	0.612482
C	0.192159	-4.478683	2.522392
C	-3.092630	-5.939236	0.019415
C	-1.808386	-7.504360	2.300152
C	-2.700094	-9.154948	-1.615986
C	0.000000	-7.965767	-2.407776

C	0.823523	-11.428837	-1.286089
C	1.427739	-9.874322	1.255652
C	-1.164782	-11.476574	1.002891
H	-1.718209	-10.930547	1.738975
H	-1.045550	9.296155	2.095735
H	1.718209	10.930547	1.738975
H	-2.174946	9.266095	0.747518
H	-1.296576	12.327872	-0.876495
H	-1.586764	10.870285	-1.818631
H	-1.937279	10.754182	1.664505
H	1.860800	11.912330	0.317072
H	-0.079973	11.744114	-2.015791
H	0.643651	12.281779	1.520077
H	3.377448	9.478756	-0.818573
H	2.562920	10.000612	-2.299460
H	3.202907	8.357131	-2.173314
H	-0.134868	8.780797	-3.127163
H	-0.994807	7.624363	-2.105201
H	0.490862	7.139441	-2.930835
H	2.605837	8.255677	2.272173
H	2.119934	6.716875	2.995552
H	0.916091	7.981342	2.719696
H	3.920675	6.656905	0.022953
H	3.014850	5.530040	-0.993157
H	3.361568	5.117039	0.690425
H	0.765757	3.986797	2.721649
H	-2.095907	6.505526	-0.387361
H	-0.984848	3.738842	2.676708
H	-0.321591	5.265610	3.273510
H	-2.035703	6.903441	1.334796
H	-2.763617	5.382382	0.802122
H	1.509345	4.456465	-2.404526
H	0.405985	3.372112	-3.256855
H	-2.588442	3.737935	-1.531705
H	-2.466847	2.544767	-0.234978
H	-2.018510	2.101691	-1.886881
H	-0.118952	5.004341	-2.822761
H	3.297975	1.425158	1.042217
H	1.072401	0.515312	-2.470324
H	2.460583	1.599362	-2.326912
H	3.168447	3.018589	0.286180
H	2.498846	0.006471	-1.558383
H	2.286539	2.672546	1.780595
H	0.804548	-1.607025	2.830383
H	1.735059	-0.103990	2.876001

H	-0.804548	1.607025	2.830383
H	-2.077506	1.316705	1.637412
H	2.077506	-1.316705	1.637412
H	-1.735059	0.103990	2.876001
H	-2.460583	-1.599362	-2.326912
H	-3.297975	-1.425158	1.042217
H	-1.072401	-0.515312	-2.470324
H	-3.168447	-3.018589	0.286180
H	-2.498846	-0.006471	-1.558383
H	-2.286539	-2.672546	1.780595
H	-0.405985	-3.372112	-3.256855
H	2.466847	-2.544767	-0.234978
H	2.588442	-3.737935	-1.531705
H	0.118952	-5.004341	-2.822761
H	2.018510	-2.101691	-1.886881
H	-1.509345	-4.456465	-2.404526
H	2.095907	-6.505526	-0.387361
H	2.763617	-5.382382	0.802122
H	0.321591	-5.265610	3.273510
H	-0.765757	-3.986797	2.721649
H	0.984848	-3.738842	2.676708
H	2.035703	-6.903441	1.334796
H	-3.014850	-5.530040	-0.993157
H	-0.916091	-7.981342	2.719696
H	-3.361568	-5.117039	0.690425
H	-3.920675	-6.656905	0.022953
H	-2.605837	-8.255677	2.272173
H	-2.119934	-6.716875	2.995552
H	-2.562920	-10.000612	-2.299460
H	-3.202907	-8.357131	-2.173314
H	-3.377448	-9.478756	-0.818573
H	0.134868	-8.780797	-3.127163
H	0.994807	-7.624363	-2.105201
H	-0.490862	-7.139441	-2.930835
H	-1.860800	-11.912330	0.317072
H	0.079973	-11.744114	-2.015791
H	1.296576	-12.327872	-0.876495
H	1.586764	-10.870285	-1.818631
H	1.937279	-10.754182	1.664505
H	1.045550	-9.296155	2.095735
H	2.174946	-9.266095	0.747518
H	-0.643651	-12.281779	1.520077

MP2/6311G optimized geometry, all-*gauche*-$Si_{13}Me_{28}$**

125
RI-MP2
Energy= -4871.64842000989665
TD B3LYP
Energy= -4882.00465311

Si	1.534174	8.769983	-1.060370
Si	1.539168	7.441656	0.881749
Si	-0.327087	6.047838	1.229078
Si	-0.994827	4.581175	-0.489148
Si	0.538912	2.981467	-1.287776
Si	1.451720	1.419282	0.220727
Si	0.000000	0.000000	1.415484
Si	-1.451720	-1.419282	0.220727
Si	-0.538912	-2.981467	-1.287776
Si	0.994827	-4.581175	-0.489148
Si	0.327087	-6.047838	1.229078
Si	-1.539168	-7.441656	0.881749
Si	-1.534174	-8.769983	-1.060370
C	2.022700	7.748565	-2.571838
C	2.845293	10.097391	-0.783356
C	-0.125846	9.643705	-1.337171
C	1.538946	8.647936	2.353086
C	3.157750	6.447385	0.938999
C	0.000000	5.080199	2.832886
C	-1.826976	7.172039	1.551359
C	-2.558269	3.704438	0.147557
C	-1.530440	5.605416	-1.999818
C	2.018159	3.881775	-2.074703
C	-0.347598	2.065414	-2.699587
C	2.465524	2.344524	1.538406
C	2.689227	0.384865	-0.786949
C	1.119037	-1.033578	2.554786
C	-1.119037	1.033578	2.554786
C	-2.465524	-2.344524	1.538406
C	-2.689227	-0.384865	-0.786949
C	0.347598	-2.065414	-2.699587
C	-2.018159	-3.881775	-2.074703
C	1.530440	-5.605416	-1.999818
C	2.558269	-3.704438	0.147557
C	1.826976	-7.172039	1.551359
C	0.000000	-5.080199	2.832886
C	-3.157750	-6.447385	0.938999
C	-1.538946	-8.647936	2.353086

C	-2.022700	-7.748565	-2.571838
C	-2.845293	-10.097391	-0.783356
C	0.125846	-9.643705	-1.337171
H	0.010443	-10.390529	-2.088703
H	2.946213	7.216059	-2.386855
H	2.579990	10.730448	0.064567
H	-0.472764	10.106795	-0.426934
H	1.255338	7.033876	-2.819453
H	3.812522	9.641759	-0.585224
H	-0.010443	10.390529	-2.088703
H	2.937566	10.723473	-1.673636
H	-0.857767	8.940405	-1.662295
H	2.173266	8.393219	-3.436513
H	3.148623	5.748307	1.776228
H	4.004684	7.124412	1.068885
H	1.581025	8.094412	3.295462
H	0.636974	9.265244	2.351976
H	2.411749	9.305615	2.305345
H	3.309217	5.893825	0.015606
H	-2.694041	6.568940	1.835743
H	-2.084946	7.748079	0.661302
H	-1.613111	7.866257	2.369117
H	0.993483	4.633023	2.816682
H	-0.749015	4.297044	2.971169
H	-0.050718	5.757336	3.691034
H	-2.830690	2.874512	-0.508589
H	-2.404546	3.332397	1.160183
H	-3.394751	4.409761	0.171339
H	-2.294202	6.332153	-1.711718
H	-1.957560	4.950903	-2.765267
H	-0.683310	6.134714	-2.434360
H	1.677064	4.663069	-2.743079
H	2.617217	3.184291	-2.653142
H	-0.450342	2.728381	-3.564270
H	0.223903	1.187339	-3.009322
H	2.652413	4.317557	-1.317320
H	-1.346716	1.758802	-2.391154
H	3.019004	3.174006	1.090991
H	2.240544	0.050923	-1.722191
H	3.565886	0.992334	-1.032186
H	3.025259	-0.482476	-0.214037
H	1.814755	2.726964	2.324657
H	3.185378	1.660904	1.999061
H	1.972279	-1.426937	2.002420
H	0.560973	-1.860575	3.000120

H	1.503267	-0.405251	3.364396
H	-1.503267	0.405251	3.364396
H	-1.972279	1.426937	2.002420
H	-0.560973	1.860575	3.000120
H	-3.565886	-0.992334	-1.032186
H	-2.240544	-0.050923	-1.722191
H	-3.025259	0.482476	-0.214037
H	-3.019004	-3.174006	1.090991
H	-3.185378	-1.660904	1.999061
H	-1.814755	-2.726964	2.324657
H	-1.677064	-4.663069	-2.743079
H	1.346716	-1.758802	-2.391154
H	0.450342	-2.728381	-3.564270
H	-0.223903	-1.187339	-3.009322
H	-2.652413	-4.317557	-1.317320
H	-2.617217	-3.184291	-2.653142
H	2.294202	-6.332153	-1.711718
H	1.957560	-4.950903	-2.765267
H	2.404546	-3.332397	1.160183
H	3.394751	-4.409761	0.171339
H	0.683310	-6.134714	-2.434360
H	2.830690	-2.874512	-0.508589
H	0.749015	-4.297044	2.971169
H	-0.993483	-4.633023	2.816682
H	0.050718	-5.757336	3.691034
H	1.613111	-7.866257	2.369117
H	2.694041	-6.568940	1.835743
H	2.084946	-7.748079	0.661302
H	-1.581025	-8.094412	3.295462
H	-0.636974	-9.265244	2.351976
H	-2.411749	-9.305615	2.305345
H	-3.309217	-5.893825	0.015606
H	-3.148623	-5.748307	1.776228
H	-4.004684	-7.124412	1.068885
H	0.857767	-8.940405	-1.662295
H	-2.946213	-7.216059	-2.386855
H	-2.173266	-8.393219	-3.436513
H	-3.812522	-9.641759	-0.585224
H	-2.579990	-10.730448	0.064567
H	-2.937566	-10.723473	-1.673636
H	-1.255338	-7.033876	-2.819453
H	0.472764	-10.106795	-0.426934

MP2/6311G optimized geometry, all-*anti*-$Si_{14}Me_{30}$**

134
RI-MP2
Energy= -5240.27418271067472
TD B3LYP
Energy= -5251.42219936

H	-1.174301	8.812452	2.462000
H	-1.174301	8.812452	-2.462000
C	-1.729440	12.879843	1.537000
H	-1.144514	12.774432	-2.457000
Si	-0.637528	12.755075	0.000000
C	0.550509	14.228240	0.000000
C	-1.729440	12.879843	-1.537000
H	-2.387649	9.740306	1.574000
H	-2.438891	7.973341	-1.556000
H	-2.387649	9.740306	-1.574000
H	-2.438891	7.973341	1.556000
H	-2.230755	13.854196	-1.574000
H	1.197506	14.224785	0.884000
H	1.197506	14.224785	-0.884000
H	-2.505983	12.108389	-1.548000
H	-0.002826	15.174629	0.000000
H	-2.505983	12.108389	1.548000
H	-1.144514	12.774432	2.457000
H	-2.230755	13.854196	1.574000
Si	0.658311	6.863189	0.000000
H	2.322789	11.781993	-1.590000
H	1.186060	10.745792	2.462000
Si	-0.658293	8.824089	0.000000
H	2.505554	10.026864	1.532000
H	2.322789	11.781993	1.590000
H	1.186060	10.745792	-2.462000
H	2.505554	10.026864	-1.532000
C	-1.767283	8.837869	-1.542000
C	-1.767283	8.837869	1.542000
Si	0.657086	10.783164	0.000000
C	1.770124	10.837381	-1.540000
C	1.770124	10.837381	1.540000
Si	-0.658311	4.902263	0.000000
H	2.387667	7.779406	-1.574000
H	1.174319	6.851552	-2.462000
Si	0.658293	2.941363	0.000000
H	2.438891	2.090615	1.556000
C	-1.767301	4.888483	1.542000

C	1.767283	2.955143	1.542000
H	-2.438909	5.753011	-1.556000
H	2.438909	6.012441	-1.556000
H	-2.387667	3.986046	1.574000
H	-1.174319	4.913900	2.462000
C	1.767301	6.876969	1.542000
C	1.767283	2.955143	-1.542000
H	1.174319	6.851552	2.462000
H	2.387649	3.857580	1.574000
H	2.387649	3.857580	-1.574000
H	2.438891	2.090615	-1.556000
Si	-0.658311	0.980463	0.000000
H	-1.174319	4.913900	-2.462000
H	2.438909	6.012441	1.556000
H	2.387667	7.779406	1.574000
H	1.174301	2.929726	-2.462000
C	1.767301	6.876969	-1.542000
C	-1.767301	4.888483	-1.542000
H	1.174301	2.929726	2.462000
H	-2.438909	5.753011	1.556000
H	-2.387667	3.986046	-1.574000
H	-1.174319	0.968826	2.462000
C	1.767301	-0.994243	-1.542000
H	-1.174319	0.968826	-2.462000
C	1.767301	-0.994243	1.542000
Si	0.658311	-0.980463	0.000000
H	-2.438909	0.129715	-1.556000
H	-2.387667	1.896680	-1.574000
H	-2.387667	1.896680	1.574000
H	2.438909	-0.129715	1.556000
H	-2.438909	0.129715	1.556000
H	1.174319	-0.968826	-2.462000
H	2.438909	-0.129715	-1.556000
C	-1.767301	0.994243	-1.542000
H	2.387667	-1.896680	-1.574000
H	1.174319	-0.968826	2.462000
C	-1.767301	0.994243	1.542000
H	2.387667	-1.896680	1.574000
Si	-0.658293	-2.941363	0.000000
H	1.174301	-8.812452	2.462000
H	1.174301	-8.812452	-2.462000
C	1.729440	-12.879843	1.537000
H	1.144514	-12.774432	-2.457000
Si	0.637528	-12.755075	0.000000
C	-0.550509	-14.228240	0.000000

C	1.729440	-12.879843	-1.537000
H	2.387649	-9.740306	1.574000
H	2.438891	-7.973341	-1.556000
H	2.387649	-9.740306	-1.574000
H	2.438891	-7.973341	1.556000
H	2.230755	-13.854196	-1.574000
H	-1.197506	-14.224785	0.884000
H	-1.197506	-14.224785	-0.884000
H	2.505983	-12.108389	-1.548000
H	0.002826	-15.174629	0.000000
H	2.505983	-12.108389	1.548000
H	1.144514	-12.774432	2.457000
H	2.230755	-13.854196	1.574000
Si	-0.658311	-6.863189	0.000000
H	-2.322789	-11.781993	-1.590000
H	-1.186060	-10.745792	2.462000
Si	0.658293	-8.824089	0.000000
H	-2.505554	-10.026864	1.532000
H	-2.322789	-11.781993	1.590000
H	-1.186060	-10.745792	-2.462000
H	-2.505554	-10.026864	-1.532000
C	1.767283	-8.837869	-1.542000
C	1.767283	-8.837869	1.542000
Si	-0.657086	-10.783164	0.000000
C	-1.770124	-10.837381	-1.540000
C	-1.770124	-10.837381	1.540000
Si	0.658311	-4.902263	0.000000
H	-2.387667	-7.779406	-1.574000
H	-1.174319	-6.851552	-2.462000
H	-2.438891	-2.090615	1.556000
C	1.767301	-4.888483	1.542000
C	-1.767283	-2.955143	1.542000
H	2.438909	-5.753011	-1.556000
H	-2.438909	-6.012441	-1.556000
H	2.387667	-3.986046	1.574000
H	1.174319	-4.913900	2.462000
C	-1.767301	-6.876969	1.542000
C	-1.767283	-2.955143	-1.542000
H	-1.174319	-6.851552	2.462000
H	-2.387649	-3.857580	1.574000
H	-2.387649	-3.857580	-1.574000
H	-2.438891	-2.090615	-1.556000
H	1.174319	-4.913900	-2.462000
H	-2.438909	-6.012441	1.556000
H	-2.387667	-7.779406	1.574000

H	-1.174301	-2.929726	-2.462000
C	-1.767301	-6.876969	-1.542000
C	1.767301	-4.888483	-1.542000
H	-1.174301	-2.929726	2.462000
H	2.438909	-5.753011	1.556000
H	2.387667	-3.986046	-1.574000

MP2/6311G optimized geometry, all-*transoid*-$Si_{14}Me_{30}$**

134
RI-MP2
Energy= -5240.28769395698146
TD B3LYP
Energy= -5251.42358292

Si	2.252201	4.288927	-0.319143
Si	4.174382	5.306416	0.578410
C	5.637787	4.107604	0.404423
C	3.918664	5.683668	2.422743
H	0.656162	5.162655	1.418217
C	0.688339	5.155397	0.323385
H	3.789612	4.761464	3.000254
C	2.300347	4.454560	-2.211026
H	0.644683	6.195652	-0.018080
H	-0.218464	4.652960	-0.031251
H	4.778282	6.218360	2.841870
H	7.090037	6.839718	2.177122
Si	4.626080	7.329013	-0.535475
H	3.031258	6.304968	2.584728
H	6.535039	4.507538	0.890301
H	5.415162	3.140046	0.867241
H	5.882571	3.924111	-0.647336
H	2.406742	5.501563	-2.514989
H	3.139577	3.897104	-2.640816
H	1.379004	4.071092	-2.663979
H	4.668867	8.709814	2.792564
H	5.514609	7.848892	-2.826419
C	5.781100	11.190371	-1.657255
H	8.694799	11.155065	1.133409
H	4.349808	10.115133	1.768073
C	7.929646	11.609441	0.494803
C	3.020557	8.311968	-0.791145
C	7.492529	7.582304	1.479450
Si	7.088100	10.320740	-0.604113
H	8.420260	12.380455	-0.110753
C	5.140613	9.460141	2.149068
H	2.505615	8.491222	0.158827
H	2.328654	7.774011	-1.448799
H	7.207625	12.110667	1.147951
H	8.050972	7.044564	0.705747
Si	6.108493	8.647866	0.730390
C	5.370891	6.935413	-2.238211
C	8.387199	9.559615	-1.745789

H	3.220344	9.287272	-1.248718
H	6.344726	6.442654	-2.145368
H	5.311124	10.499746	-2.365583
H	8.208097	8.200061	2.034433
H	5.801461	10.068391	2.776841
H	6.228056	12.005096	-2.239040
H	9.180971	9.068055	-1.173263
H	8.857613	10.329140	-2.368963
H	7.949015	8.812233	-2.414943
H	4.987435	11.623739	-1.039089
Si	2.155258	2.023846	0.309889
H	4.716431	6.271730	-2.813655
Si	-2.252201	-4.288927	-0.319143
Si	-4.174382	-5.306416	0.578410
C	-5.637787	-4.107604	0.404423
C	-3.918664	-5.683668	2.422743
H	-0.656162	-5.162655	1.418217
C	-0.688339	-5.155397	0.323385
H	-3.789612	-4.761464	3.000254
C	-2.300347	-4.454560	-2.211026
H	-0.644683	-6.195652	-0.018080
H	0.218464	-4.652960	-0.031251
H	-4.778282	-6.218360	2.841870
H	-7.090037	-6.839718	2.177122
Si	-4.626080	-7.329013	-0.535475
H	-3.031258	-6.304968	2.584728
H	-6.535039	-4.507538	0.890301
H	-5.415162	-3.140046	0.867241
H	-5.882571	-3.924111	-0.647336
H	-2.406742	-5.501563	-2.514989
H	-3.139577	-3.897104	-2.640816
H	-1.379004	-4.071092	-2.663979
H	-4.668867	-8.709814	2.792564
H	-5.514609	-7.848892	-2.826419
C	-5.781100	-11.190371	-1.657255
H	-8.694799	-11.155065	1.133409
H	-4.349808	-10.115133	1.768073
C	-7.929646	-11.609441	0.494803
C	-3.020557	-8.311968	-0.791145
C	-7.492529	-7.582304	1.479450
Si	-7.088100	-10.320740	-0.604113
H	-8.420260	-12.380455	-0.110753
C	-5.140613	-9.460141	2.149068
H	-2.505615	-8.491222	0.158827
H	-2.328654	-7.774011	-1.448799

H	-7.207625	-12.110667	1.147951
H	-8.050972	-7.044564	0.705747
Si	-6.108493	-8.647866	0.730390
C	-5.370891	-6.935413	-2.238211
C	-8.387199	-9.559615	-1.745789
H	-3.220344	-9.287272	-1.248718
H	-6.344726	-6.442654	-2.145368
H	-5.311124	-10.499746	-2.365583
H	-8.208097	-8.200061	2.034433
H	-5.801461	-10.068391	2.776841
H	-6.228056	-12.005096	-2.239040
H	-9.180971	-9.068055	-1.173263
H	-8.857613	-10.329140	-2.368963
H	-7.949015	-8.812233	-2.414943
H	-4.987435	-11.623739	-1.039089
Si	-2.155258	-2.023846	0.309889
H	-4.716431	-6.271730	-2.813655
H	-0.109359	1.455140	-2.512959
H	-2.163311	1.319620	1.284476
H	3.294298	-0.072982	-0.478789
H	-1.280165	2.848644	1.369556
C	3.373582	0.992553	-0.720205
H	3.185832	1.104707	-1.793497
C	-0.688339	1.834708	-1.664140
H	2.700845	0.842975	2.458896
H	3.629293	2.341033	2.321407
H	4.408562	1.298348	-0.529430
Si	-0.015546	1.176297	-0.014044
Si	0.015546	-1.176297	-0.014044
H	-0.773547	1.477207	2.365882
H	-1.732013	1.534857	-1.812197
H	-0.651003	2.928916	-1.699462
C	-1.164419	1.759114	1.382270
H	1.924674	2.398658	2.786885
C	2.647431	1.889900	2.139944
H	-3.185832	-1.104707	-1.793497
H	-3.629293	-2.341033	2.321407
H	0.651003	-2.928916	-1.699462
H	-2.700845	-0.842975	2.458896
C	0.688339	-1.834708	-1.664140
H	0.109359	-1.455140	-2.512959
C	-3.373582	-0.992553	-0.720205
H	1.280165	-2.848644	1.369556
H	2.163311	-1.319620	1.284476
H	1.732013	-1.534857	-1.812197

H	-1.924674	-2.398658	2.786885
H	-4.408562	-1.298348	-0.529430
H	-3.294298	0.072982	-0.478789
C	-2.647431	-1.889900	2.139944
H	0.773547	-1.477207	2.365882
C	1.164419	-1.759114	1.382270

MP2/6311G optimized geometry, all-*deviant*-$Si_{14}Me_{30}$**

134
RI-MP2
Energy= -5240.26828067982024
TD B3LYP
Energy= -5251.40831215

H	2.844454	4.541077	0.050974
H	-2.786857	11.627304	-0.191587
H	3.025909	11.724215	-0.460499
Si	0.392749	4.848158	0.603816
H	0.739345	9.594452	2.807238
C	2.256143	4.686820	0.974516
C	1.646580	6.892383	-1.856733
H	-2.176163	12.439497	-1.662803
H	-1.331684	5.946997	-2.586149
H	-1.587466	5.216130	2.134763
H	1.728422	5.967992	-2.459165
H	0.920897	11.558182	-2.799387
H	-1.579464	7.696336	-2.322141
H	-0.468978	3.996171	2.809462
H	-0.403453	10.363158	-2.684529
H	1.855066	8.374547	2.127870
H	3.150099	9.947848	-0.295907
H	0.338527	7.857462	2.923377
H	2.453825	3.831808	1.646649
H	2.626353	5.602605	1.472919
H	-2.795313	13.412886	-0.297710
C	-0.520857	4.963392	2.275167
C	0.376189	14.138977	-0.458666
C	-0.626563	12.716229	2.078393
H	1.295447	9.813351	-2.765404
Si	0.127996	6.795434	-0.707739
H	-2.333996	6.512036	-1.216404
C	-1.427590	6.727210	-1.810858
H	-0.067686	5.733152	2.924099
H	2.584147	7.009076	-1.284340
H	1.561463	7.745253	-2.554770
Si	-0.484414	2.922591	-0.447435
H	2.703808	10.946933	1.118701
Si	-0.131396	8.742639	0.605066
C	-1.993258	8.903947	0.983399
C	0.789039	8.627274	2.272657
Si	0.741799	10.669042	-0.450021
C	-2.224040	12.502624	-0.560473

H	-1.177113	13.633326	2.360825
H	1.384548	14.251455	-0.020788
Si	-0.484900	12.576637	0.191600
C	2.578423	10.838028	0.026585
C	0.626563	10.589456	-2.353943
H	-0.209863	15.041091	-0.199930
H	-1.164428	11.851824	2.508004
H	0.372388	12.762805	2.549276
H	-2.188190	9.758906	1.656403
H	-2.361426	7.988122	1.483238
H	-2.585343	9.049762	0.062284
H	0.483567	14.108392	-1.558123
H	-2.844454	-4.541077	0.050974
H	2.786857	-11.627304	-0.191587
H	-3.025909	-11.724215	-0.460499
Si	-0.392749	-4.848158	0.603816
H	-0.739345	-9.594452	2.807238
C	-2.256143	-4.686820	0.974516
C	-1.646580	-6.892383	-1.856733
H	2.176163	-12.439497	-1.662803
H	1.331684	-5.946997	-2.586149
H	1.587466	-5.216130	2.134763
H	-1.728422	-5.967992	-2.459165
H	-0.920897	-11.558182	-2.799387
H	1.579464	-7.696336	-2.322141
H	0.468978	-3.996171	2.809462
H	0.403453	-10.363158	-2.684529
H	-1.855066	-8.374547	2.127870
H	-3.150099	-9.947848	-0.295907
H	-0.338527	-7.857462	2.923377
H	-2.453825	-3.831808	1.646649
H	-2.626353	-5.602605	1.472919
H	2.795313	-13.412886	-0.297710
C	0.520857	-4.963392	2.275167
C	-0.376189	-14.138977	-0.458666
C	0.626563	-12.716229	2.078393
H	-1.295447	-9.813351	-2.765404
Si	-0.127996	-6.795434	-0.707739
H	2.333996	-6.512036	-1.216404
C	1.427590	-6.727210	-1.810858
H	0.067686	-5.733152	2.924099
H	-2.584147	-7.009076	-1.284340
H	-1.561463	-7.745253	-2.554770
Si	0.484414	-2.922591	-0.447435
H	-2.703808	-10.946933	1.118701

Si	0.131396	-8.742639	0.605066
C	1.993258	-8.903947	0.983399
C	-0.789039	-8.627274	2.272657
Si	-0.741799	-10.669042	-0.450021
C	2.224040	-12.502624	-0.560473
H	1.177113	-13.633326	2.360825
H	-1.384548	-14.251455	-0.020788
Si	0.484900	-12.576637	0.191600
C	-2.578423	-10.838028	0.026585
C	-0.626563	-10.589456	-2.353943
H	0.209863	-15.041091	-0.199930
H	1.164428	-11.851824	2.508004
H	-0.372388	-12.762805	2.549276
H	2.188190	-9.758906	1.656403
H	2.361426	-7.988122	1.483238
H	2.585343	-9.049762	0.062284
H	-0.483567	-14.108392	-1.558123
H	1.024858	-3.909990	-2.706073
H	1.869527	0.067146	2.173319
C	-0.432616	3.047467	-2.349384
H	2.770393	1.715360	-1.054666
H	2.222093	1.805055	1.957333
H	2.869077	-2.091765	-0.492949
H	2.805137	-3.835168	-0.108587
H	-0.652832	-1.288975	2.643653
H	-2.222093	-1.805055	1.957333
H	-1.869527	-0.067146	2.173319
C	0.432616	-3.047467	-2.349384
C	2.317919	-2.859659	0.077639
H	0.600784	3.162335	-2.722443
C	-2.317919	2.859659	0.077639
H	0.652832	1.288975	2.643653
H	1.788540	0.676678	-2.128649
H	2.421287	-2.629196	1.153486
H	0.858627	-2.132743	-2.803193
H	-1.788540	-0.676678	-2.128649
H	-0.858627	2.132743	-2.803193
H	-2.785647	0.059012	-0.837823
H	2.785647	-0.059012	-0.837823
Si	0.691286	0.957972	0.135793
H	-2.770393	-1.715360	-1.054666
H	-2.869077	2.091765	-0.492949
C	2.143403	0.804464	-1.090369
H	-2.421287	2.629196	1.153486
H	-1.024858	3.909990	-2.706073

C	-1.426808	-1.041810	1.894576
H	-2.805137	3.835168	-0.108587
C	1.426808	1.041810	1.894576
Si	-0.691286	-0.957972	0.135793
C	-2.143403	-0.804464	-1.090369
H	-0.600784	-3.162335	-2.722443

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{14}Me_{30}$**

134
RI-MP2
Energy= -5240.23614637754054
TD B3LYP
Energy= -5251.37975906

C	1.137722	6.649333	-1.536952
H	0.580665	6.365186	-2.446065
H	-1.928743	9.786114	-2.695053
H	-3.376125	5.017746	-0.158709
H	-0.822422	3.551399	2.866921
H	1.718223	8.246832	1.158290
H	-0.634031	5.313070	3.097724
H	-2.896830	11.784589	2.300063
H	-3.212601	10.025550	2.330051
C	-2.151487	12.891778	-1.725689
H	0.614626	7.505906	2.354984
H	-3.187901	5.666638	1.496513
C	-2.884800	4.851551	0.815210
H	-3.265918	3.900625	1.231658
H	1.918471	5.887986	-1.360338
H	1.641467	7.614056	-1.733149
C	0.870098	12.305670	-1.402842
Si	-0.986196	4.762989	0.665678
H	-0.196412	9.364251	-2.553505
Si	0.003525	6.823897	-0.014446
H	-3.635534	7.840421	0.640686
H	-1.390594	8.106184	-2.978743
H	-3.547225	7.222645	-1.034665
H	-0.403225	14.892752	0.141512
Si	-0.517766	2.866099	-0.702546
H	1.692997	12.078170	-0.700860
H	1.907845	6.527691	1.606445
H	0.735300	4.343418	2.485895
C	-0.361205	4.462895	2.445461
C	1.165834	7.325078	1.415992
H	-1.553699	14.125202	1.274021
H	-3.974985	8.931753	-0.732993
Si	-0.777268	12.491455	-0.481697
Si	-1.276270	10.575556	0.802328
Si	-1.504126	8.603866	-0.512799
H	-1.925491	13.839110	-2.250404
H	0.199350	13.811062	1.430891
C	-0.619609	13.965688	0.705427

C	0.035046	10.472079	2.182274
C	-2.949395	10.875080	1.672982
C	-3.337557	8.095420	-0.390684
C	-1.222042	9.006016	-2.358605
H	-3.124683	13.011348	-1.215819
H	0.827131	11.497543	-2.154111
H	-2.259052	12.099692	-2.487375
H	1.123718	13.245802	-1.927865
H	1.055814	10.356606	1.778434
H	-0.160102	9.623208	2.861703
H	0.007075	11.400873	2.782009
H	-3.770348	11.007522	0.946070
C	-1.137722	-6.649333	-1.536952
H	-0.580665	-6.365186	-2.446065
H	1.928743	-9.786114	-2.695053
H	3.376125	-5.017746	-0.158709
H	0.822422	-3.551399	2.866921
H	-1.718223	-8.246832	1.158290
H	0.634031	-5.313070	3.097724
H	2.896830	-11.784589	2.300063
H	3.212601	-10.025550	2.330051
C	2.151487	-12.891778	-1.725689
H	-0.614626	-7.505906	2.354984
H	3.187901	-5.666638	1.496513
C	2.884800	-4.851551	0.815210
H	3.265918	-3.900625	1.231658
H	-1.918471	-5.887986	-1.360338
H	-1.641467	-7.614056	-1.733149
C	-0.870098	-12.305670	-1.402842
Si	0.986196	-4.762989	0.665678
H	0.196412	-9.364251	-2.553505
Si	-0.003525	-6.823897	-0.014446
H	3.635534	-7.840421	0.640686
H	1.390594	-8.106184	-2.978743
H	3.547225	-7.222645	-1.034665
H	0.403225	-14.892752	0.141512
Si	0.517766	-2.866099	-0.702546
H	-1.692997	-12.078170	-0.700860
H	-1.907845	-6.527691	1.606445
H	-0.735300	-4.343418	2.485895
C	0.361205	-4.462895	2.445461
C	-1.165834	-7.325078	1.415992
H	1.553699	-14.125202	1.274021
H	3.974985	-8.931753	-0.732993
Si	0.777268	-12.491455	-0.481697

Si	1.276270	-10.575556	0.802328
Si	1.504126	-8.603866	-0.512799
H	1.925491	-13.839110	-2.250404
H	-0.199350	-13.811062	1.430891
C	0.619609	-13.965688	0.705427
C	-0.035046	-10.472079	2.182274
C	2.949395	-10.875080	1.672982
C	3.337557	-8.095420	-0.390684
C	1.222042	-9.006016	-2.358605
H	3.124683	-13.011348	-1.215819
H	-0.827131	-11.497543	-2.154111
H	2.259052	-12.099692	-2.487375
H	-1.123718	-13.245802	-1.927865
H	-1.055814	-10.356606	1.778434
H	0.160102	-9.623208	2.861703
H	-0.007075	-11.400873	2.782009
H	3.770348	-11.007522	0.946070
C	-0.619609	-3.364474	-2.153855
C	1.035274	1.393445	2.185405
H	-2.575001	3.240518	-2.076859
H	-2.865663	-0.067192	-0.060490
H	2.128668	0.601035	-1.600238
C	-2.172295	2.377778	-1.514320
H	0.154309	4.171730	-2.748001
H	-2.030382	1.544557	-2.225665
C	2.172295	-2.377778	-1.514320
H	-2.828288	-1.803463	-0.480269
H	0.786260	2.502354	-2.825907
H	0.144037	1.514646	2.824581
Si	0.583083	1.040398	0.367224
H	2.865663	0.067192	-0.060490
H	2.030382	-1.544557	-2.225665
H	2.575001	-3.240518	-2.076859
Si	-0.583083	-1.040398	0.367224
C	0.619609	3.364474	-2.153855
H	2.828288	1.803463	-0.480269
C	-1.035274	-1.393445	2.185405
H	-1.644654	-2.311194	2.267886
H	1.605599	3.718251	-1.806148
C	2.256958	0.858313	-0.534600
H	-2.930064	2.071050	-0.773210
H	-1.605599	-3.718251	-1.806148
C	-2.256958	-0.858313	-0.534600
H	1.644654	2.311194	2.267886
H	-1.630858	-0.552406	2.586497

H	-2.128668	-0.601035	-1.600238
H	2.930064	-2.071050	-0.773210
H	1.630858	0.552406	2.586497
H	-0.144037	-1.514646	2.824581
H	-0.154309	-4.171730	-2.748001
H	-0.786260	-2.502354	-2.825907

MP2/6311G optimized geometry, all-*ortho*-$Si_{14}Me_{30}$**

134
RI-MP2
Energy= -5240.27645739143009
TD B3LYP
Energy= -5251.41075648

H	-3.306030	9.365767	-2.762667
Si	-3.300600	7.075566	0.430376
C	-4.987307	7.309791	-0.417559
C	-3.641431	6.228406	2.096620
Si	-2.357304	9.194047	0.862913
H	-4.138983	9.826298	2.531364
H	-5.426937	10.421833	-0.715045
H	-1.632856	9.933675	-2.694683
Si	-2.948600	10.811320	-0.744695
C	-3.044316	9.789798	2.534164
C	-0.466969	9.116952	1.028059
H	-2.183870	13.158760	-1.147676
H	-0.831560	12.150843	-0.616115
H	-2.917287	11.025809	-3.228206
H	-5.642040	7.957570	0.176633
H	-5.496920	6.347441	-0.540259
H	-4.886899	7.759315	-1.411403
Si	-1.989155	5.691746	-0.960749
H	-2.680016	10.794931	2.776077
H	-2.736899	9.121816	3.346249
C	-2.673215	10.225730	-2.519387
C	-4.768122	11.277810	-0.537996
C	-1.895552	12.356409	-0.458553
H	-4.329748	6.832820	2.698120
H	-2.725721	6.091147	2.681119
H	-4.097948	5.243044	1.957570
H	-4.972327	11.652369	0.470610
H	-2.011893	12.739952	0.560849
H	-5.049281	12.065843	-1.246318
H	-0.063594	10.104103	1.280785
H	0.013768	8.790087	0.100277
H	-0.167984	8.424117	1.821424
H	-3.770490	3.938716	-1.305918
C	-1.067405	6.776865	-2.222387
C	-3.159745	4.573914	-1.955931
H	-0.418821	5.564360	2.427881
H	-3.373263	1.605363	1.951524
C	-3.001770	2.522658	1.480948

H	-0.334533	7.432703	-1.740045
H	-2.604713	3.918525	-2.634965
C	-0.222549	1.908838	2.576863
H	0.854560	1.824228	2.398872
C	1.067405	4.092789	-1.011200
H	-3.842729	5.180068	-2.561744
H	1.151448	4.811674	2.126233
H	1.525549	5.038349	-1.322484
H	-0.372311	2.688932	3.331796
H	-3.135702	3.340325	2.198471
H	-0.564240	0.960933	3.005121
H	0.741718	3.569778	-1.916885
Si	-1.174029	2.334438	0.988227
H	-3.639667	2.731342	0.615259
H	1.848635	3.486274	-0.538784
H	-1.764315	7.410885	-2.782469
H	0.738741	6.342438	1.341395
Si	-1.034071	0.568473	-0.571212
H	-0.528700	6.156482	-2.947508
C	0.336249	5.374699	1.657881
Si	-0.376654	4.406168	0.186850
H	3.306030	-9.365767	-2.762667
Si	3.300600	-7.075566	0.430376
C	4.987307	-7.309791	-0.417559
C	3.641431	-6.228406	2.096620
Si	2.357304	-9.194047	0.862913
H	4.138983	-9.826298	2.531364
H	5.426937	-10.421833	-0.715045
H	1.632856	-9.933675	-2.694683
Si	2.948600	-10.811320	-0.744695
C	3.044316	-9.789798	2.534164
C	0.466969	-9.116952	1.028059
H	2.183870	-13.158760	-1.147676
H	0.831560	-12.150843	-0.616115
H	2.917287	-11.025809	-3.228206
H	5.642040	-7.957570	0.176633
H	5.496920	-6.347441	-0.540259
H	4.886899	-7.759315	-1.411403
Si	1.989155	-5.691746	-0.960749
H	2.680016	-10.794931	2.776077
H	2.736899	-9.121816	3.346249
C	2.673215	-10.225730	-2.519387
C	4.768122	-11.277810	-0.537996
C	1.895552	-12.356409	-0.458553
H	4.329748	-6.832820	2.698120

H	2.725721	-6.091147	2.681119
H	4.097948	-5.243044	1.957570
H	4.972327	-11.652369	0.470610
H	2.011893	-12.739952	0.560849
H	5.049281	-12.065843	-1.246318
H	0.063594	-10.104103	1.280785
H	-0.013768	-8.790087	0.100277
H	0.167984	-8.424117	1.821424
H	3.770490	-3.938716	-1.305918
C	1.067405	-6.776865	-2.222387
C	3.159745	-4.573914	-1.955931
H	0.418821	-5.564360	2.427881
H	3.373263	-1.605363	1.951524
C	3.001770	-2.522658	1.480948
H	0.334533	-7.432703	-1.740045
H	2.604713	-3.918525	-2.634965
C	0.222549	-1.908838	2.576863
H	-0.854560	-1.824228	2.398872
C	-1.067405	-4.092789	-1.011200
H	3.842729	-5.180068	-2.561744
H	-1.151448	-4.811674	2.126233
H	-1.525549	-5.038349	-1.322484
H	0.372311	-2.688932	3.331796
H	3.135702	-3.340325	2.198471
H	0.564240	-0.960933	3.005121
H	-0.741718	-3.569778	-1.916885
Si	1.174029	-2.334438	0.988227
H	3.639667	-2.731342	0.615259
H	-1.848635	-3.486274	-0.538784
H	1.764315	-7.410885	-2.782469
H	-0.738741	-6.342438	1.341395
Si	1.034071	-0.568473	-0.571212
H	0.528700	-6.156482	-2.947508
C	-0.336249	-5.374699	1.657881
Si	0.376654	-4.406168	0.186850
H	-2.461110	-1.469457	-0.940834
H	-3.427741	-0.119387	-0.330531
C	-2.465407	-0.634416	-0.232760
H	3.427741	0.119387	-0.330531
H	1.349722	-0.453833	-3.057845
H	-2.251889	1.817009	-2.383045
C	1.307849	-1.263604	-2.320691
H	2.417065	1.054616	0.777239
H	-0.503019	1.942914	-2.621799
C	2.465407	0.634416	-0.232760

H	2.251889	-1.817009	-2.383045
H	2.461110	1.469457	-0.940834
C	-1.307849	1.263604	-2.320691
H	-2.417065	-1.054616	0.777239
H	-1.349722	0.453833	-3.057845
H	0.503019	-1.942914	-2.621799

MP2/6311G optimized geometry, all-*gauche*-$Si_{14}Me_{30}$**

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RI-MP2
Energy= -5240.27360293612401
TD B3LYP
Energy= -5251.40125908

H	2.091974	4.517058	-0.930902
H	-3.165178	2.983483	1.699125
H	-1.864428	3.680726	2.697920
H	-3.449746	4.456998	2.639831
H	2.159297	7.200147	-0.372673
H	-4.234437	6.360529	0.560696
H	-4.409848	4.940644	-0.482956
Si	0.759819	2.413278	-0.623883
H	0.371813	0.996797	-2.651699
C	-2.586284	2.393026	-1.597275
H	-1.751431	5.180069	-2.964327
H	-0.507154	4.023266	-3.457527
C	-2.707746	3.912393	2.047689
C	-3.722886	5.735440	-0.176794
H	-3.363093	2.921508	-2.158589
H	1.952447	8.565992	-1.484261
H	-3.488728	6.342814	-1.051550
H	1.575822	2.248268	-2.975607
C	2.153902	3.656025	-0.260038
C	1.232298	1.519612	-2.234778
C	-0.846083	4.662915	-2.637039
H	-2.186190	1.599612	-2.232883
Si	0.771142	0.890322	1.173282
C	-0.883387	11.102693	-1.816286
H	2.041004	0.806550	-2.058072
H	2.100437	4.000334	0.772731
H	-0.069859	5.397807	-2.430701
H	3.126294	3.175710	-0.406442
Si	-1.213093	3.610874	-1.095819
H	-3.050449	1.953501	-0.714787
C	-1.879446	8.385632	-2.869431
H	-0.933007	8.207150	-3.388141
Si	-0.847634	6.721156	1.488754
H	1.413652	9.327667	1.893098
H	-0.721419	11.732025	-0.936323
H	-3.015202	10.248621	0.568946
H	-2.326353	7.423084	-2.620139
C	0.617203	6.021486	2.479490

Si	0.000000	8.385745	0.055619
C	-2.001344	7.604967	2.716801
H	0.071208	10.973622	-2.334878
H	-3.921909	10.251874	-0.955034
C	-3.206607	9.686839	-0.350015
C	1.437180	7.731218	-0.999402
Si	-1.604635	9.426874	-1.317459
C	0.671152	9.744879	1.206315
H	-1.572538	11.623076	-2.488001
H	-3.664605	8.731169	-0.086523
H	-0.136827	10.191567	1.793126
H	-2.353643	6.900771	3.476594
H	-2.870781	8.026279	2.205697
H	-1.468933	8.414329	3.224890
H	1.435407	5.745437	1.814348
H	0.309476	5.147070	3.058282
H	0.989111	6.779505	3.175734
H	-2.553672	8.906635	-3.555680
H	1.152871	10.533025	0.620038
Si	-2.147511	4.980713	0.577426
H	1.081598	7.055209	-1.776246
Si	-0.771142	-0.890322	1.173282
C	-0.469013	-1.825017	2.802795
C	-2.546761	-0.214970	1.262391
H	2.897997	-0.077297	0.272943
C	2.546761	0.214970	1.262391
H	2.601649	-0.642761	1.936793
C	0.469013	1.825017	2.802795
H	3.218713	0.991199	1.641733
H	-3.218713	-0.991199	1.641733
H	-2.897997	0.077297	0.272943
H	-2.601649	0.642761	1.936793
Si	-0.759819	-2.413278	-0.623883
H	-0.988722	-2.786149	2.801046
H	-0.845720	-1.233798	3.643286
H	0.596986	-1.989313	2.959652
H	0.845720	1.233798	3.643286
H	-0.596986	1.989313	2.959652
H	0.988722	2.786149	2.801046
H	-2.091974	-4.517058	-0.930902
H	3.165178	-2.983483	1.699125
H	1.864428	-3.680726	2.697920
H	3.449746	-4.456998	2.639831
H	-2.159297	-7.200147	-0.372673
H	4.234437	-6.360529	0.560696

H	4.409848	-4.940644	-0.482956
H	-0.371813	-0.996797	-2.651699
C	2.586284	-2.393026	-1.597275
H	1.751431	-5.180069	-2.964327
H	0.507154	-4.023266	-3.457527
C	2.707746	-3.912393	2.047689
C	3.722886	-5.735440	-0.176794
H	3.050449	-1.953501	-0.714787
H	-1.952447	-8.565992	-1.484261
H	3.488728	-6.342814	-1.051550
H	-1.575822	-2.248268	-2.975607
C	-2.153902	-3.656025	-0.260038
C	-1.232298	-1.519612	-2.234778
C	0.846083	-4.662915	-2.637039
H	3.363093	-2.921508	-2.158589
C	0.883387	-11.102693	-1.816286
H	-2.041004	-0.806550	-2.058072
H	-2.100437	-4.000334	0.772731
H	0.069859	-5.397807	-2.430701
H	-3.126294	-3.175710	-0.406442
Si	1.213093	-3.610874	-1.095819
H	2.186190	-1.599612	-2.232883
C	1.879446	-8.385632	-2.869431
H	0.933007	-8.207150	-3.388141
Si	0.847634	-6.721156	1.488754
H	-1.413652	-9.327667	1.893098
H	0.721419	-11.732025	-0.936323
H	3.015202	-10.248621	0.568946
H	2.326353	-7.423084	-2.620139
C	-0.617203	-6.021486	2.479490
Si	0.000000	-8.385745	0.055619
C	2.001344	-7.604967	2.716801 -
H	-0.071208	-10.973622	-2.334878
H	3.921909	-10.251874	-0.955034
C	3.206607	-9.686839	-0.350015
C	-1.437180	-7.731218	-0.999402
Si	1.604635	-9.426874	-1.317459
C	-0.671152	-9.744879	1.206315
H	1.572538	-11.623076	-2.488001
H	3.664605	-8.731169	-0.086523
H	0.136827	-10.191567	1.793126
H	2.353643	-6.900771	3.476594
H	2.870781	-8.026279	2.205697
H	1.468933	-8.414329	3.224890
H	-1.435407	-5.745437	1.814348

H	-0.309476	-5.147070	3.058282
H	-0.989111	-6.779505	3.175734
H	2.553672	-8.906635	-3.555680
H	-1.152871	-10.533025	0.620038
Si	2.147511	-4.980713	0.577426
H	-1.081598	-7.055209	-1.776246

MP2/6311G optimized geometry, all-*anti*-$Si_{15}Me_{32}$**

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RI-MP2
Energy= -5608.89142575799815
TD B3LYP
Energy= -5620.81485931

Si	0.000000	-13.731327	-0.586254
Si	0.000000	-11.760750	0.710390
Si	0.000000	-9.800322	-0.602972
Si	0.000000	-7.840778	0.715650
Si	0.000000	-5.878498	-0.598953
Si	0.000000	-3.918954	0.719669
Si	0.000000	-1.956700	-0.594915
Si	0.000000	0.000000	0.723725
Si	0.000000	1.956700	-0.594915
Si	0.000000	3.918954	0.719669
Si	0.000000	5.878498	-0.598953
Si	0.000000	7.840778	0.715650
Si	0.000000	9.800322	-0.602972
Si	0.000000	11.760750	0.710390
Si	0.000000	13.731327	-0.586254
C	1.537000	-13.854971	-1.678294
C	0.000000	-15.205714	0.600266
C	-1.537000	-13.854971	-1.678294
C	1.540000	-11.816113	1.823371
C	-1.540000	-11.816113	1.823371
C	-1.542000	-9.812960	-1.711976
C	1.542000	-9.812960	-1.711976
C	-1.542000	-7.855700	1.824625
C	1.542000	-7.855700	1.824625
C	-1.542000	-5.863576	-1.707928
C	1.542000	-5.863576	-1.707928
C	1.542000	-3.933876	1.828645
C	-1.542000	-3.933876	1.828645
C	-1.542000	-1.969338	-1.703919
C	1.542000	-1.969338	-1.703919
C	-1.542000	0.000000	1.832728
C	1.542000	0.000000	1.832728
C	-1.542000	1.969338	-1.703919
C	1.542000	1.969338	-1.703919
C	-1.542000	3.933876	1.828645
C	1.542000	3.933876	1.828645
C	1.542000	5.863576	-1.707928
C	-1.542000	5.863576	-1.707928

C	-1.542000	7.855700	1.824625
C	1.542000	7.855700	1.824625
C	1.542000	9.812960	-1.711976
C	-1.542000	9.812960	-1.711976
C	-1.540000	11.816113	1.823371
C	1.540000	11.816113	1.823371
C	1.537000	13.854971	-1.678294
C	-1.537000	13.854971	-1.678294
C	0.000000	15.205714	0.600266
H	-0.884000	15.202925	1.247266
H	1.574000	1.050688	-2.321158
H	2.462000	-9.788153	-1.118968
H	-2.462000	-9.788153	-1.118968
H	-2.457000	-13.750162	-1.093259
H	1.574000	-10.714758	-2.333270
H	-1.556000	-8.947741	-2.382693
H	-1.574000	-10.714758	-2.333270
H	1.556000	-8.947741	-2.382693
H	-1.574000	-14.828807	-2.180611
H	0.884000	-15.202925	1.247266
H	-0.884000	-15.202925	1.247266
H	-1.548000	-13.082718	-2.454042
H	0.000000	-16.151534	0.045957
H	1.548000	-13.082718	-2.454042
H	2.457000	-13.750162	-1.093259
H	1.574000	-14.828807	-2.180611
H	-1.590000	-12.761293	2.375063
H	2.462000	-11.723922	1.239402
H	1.532000	-11.006353	2.559635
H	1.590000	-12.761293	2.375063
H	-2.462000	-11.723922	1.239402
H	-1.532000	-11.006353	2.559635
H	-1.574000	-8.758775	2.444062
H	-2.462000	-7.829672	1.231670
H	1.556000	-3.070039	2.501142
H	-1.556000	-6.727412	-2.380426
H	-1.556000	-6.991863	2.497123
H	1.574000	-4.960501	-2.327365
H	2.462000	-5.889603	-1.114972
H	2.462000	-7.829672	1.231670
H	1.574000	-4.836951	2.448081
H	-1.574000	-4.836951	2.448081
H	-1.556000	-3.070039	2.501142
H	-2.462000	-5.889603	-1.114972
H	1.556000	-6.991863	2.497123

H	1.574000	-8.758775	2.444062
H	-2.462000	-3.907848	1.235689
H	2.462000	-3.907848	1.235689
H	1.556000	-6.727412	-2.380426
H	-1.574000	-4.960501	-2.327365
H	2.462000	11.723922	1.239402
H	-2.462000	11.723922	1.239402
H	1.590000	12.761293	2.375063
H	-1.532000	11.006353	2.559635
H	-1.590000	12.761293	2.375063
H	1.532000	11.006353	2.559635
H	-1.574000	14.828807	-2.180611
H	2.457000	13.750162	-1.093259
H	1.548000	13.082718	-2.454042
H	1.574000	14.828807	-2.180611
H	-2.457000	13.750162	-1.093259
H	-1.548000	13.082718	-2.454042
H	-1.574000	10.714758	-2.333270
H	-2.462000	9.788153	-1.118968
H	1.574000	4.960501	-2.327365
H	-1.574000	8.758775	2.444062
H	-1.556000	8.947741	-2.382693
H	1.556000	6.991863	2.497123
H	2.462000	7.829672	1.231670
H	2.462000	9.788153	-1.118968
H	1.556000	6.727412	-2.380426
H	-1.556000	6.727412	-2.380426
H	-1.574000	4.960501	-2.327365
H	-2.462000	7.829672	1.231670
H	1.556000	8.947741	-2.382693
H	1.574000	10.714758	-2.333270
H	-2.462000	5.889603	-1.114972
H	2.462000	5.889603	-1.114972
H	1.574000	8.758775	2.444062
H	-1.556000	6.991863	2.497123
H	2.462000	-1.944531	-1.110911
H	-2.462000	-1.944531	-1.110911
H	-1.574000	-1.050688	-2.321158
H	-1.574000	-2.871136	-2.325214
H	1.574000	-2.871136	-2.325214
H	1.556000	-0.849711	2.503446
H	1.574000	-1.050688	-2.321158
H	-2.462000	0.000000	1.239720
H	-1.556000	-0.849711	2.503446
H	-1.556000	0.849711	2.503446

H	2.462000	0.000000	1.239720
H	1.556000	0.849711	2.503446
H	2.462000	3.907848	1.235689
H	-2.462000	3.907848	1.235689
H	-1.556000	3.070039	2.501142
H	-1.574000	4.836951	2.448081
H	1.574000	4.836951	2.448081
H	1.574000	2.871136	-2.325214
H	1.556000	3.070039	2.501142
H	-2.462000	1.944531	-1.110911
H	-1.574000	2.871136	-2.325214
H	-1.574000	1.050688	-2.321158
H	2.462000	1.944531	-1.110911
H	0.884000	15.202925	1.247266
H	0.000000	16.151534	0.045957

MP2/6311G optimized geometry, all-*transoid*-$Si_{15}Me_{32}$**

143
RI-MP2
Energy= -5608.89040208888855
TD B3LYP
Energy= -5620.80099024

Si	0.000000	-13.496991	0.086250
Si	1.244051	-11.499175	0.076162
Si	-0.159922	-9.640973	-0.263368
Si	0.934070	-7.659796	0.379898
Si	-0.161883	-5.786964	-0.529526
Si	0.497214	-3.827332	0.593463
Si	-0.061794	-1.927909	-0.677506
Si	0.000000	0.000000	0.667824
Si	0.061794	1.927909	-0.677506
Si	-0.497214	3.827332	0.593463
Si	0.161883	5.786964	-0.529526
Si	-0.934070	7.659796	0.379898
Si	0.159922	9.640973	-0.263368
Si	-1.244051	11.499175	0.076162
Si	0.000000	13.496991	0.086250
C	-1.216543	-13.537539	-1.360122
C	1.163673	-14.980064	-0.065164
C	-0.965803	-13.649703	1.703128
C	2.171679	-11.354506	1.728629
C	2.522693	-11.560402	-1.327605
C	-1.755244	-9.815448	0.753234
C	-0.621962	-9.569168	-2.104736
C	0.957215	-7.494610	2.272291
C	2.727666	-7.738342	-0.241485
C	0.275137	-5.597910	-2.368696
C	-2.038035	-6.043952	-0.377904
C	-0.361799	-3.705806	2.283522
C	2.374692	-3.901761	0.874197
C	-1.801280	-2.181340	-1.398088
C	1.160340	-1.703247	-2.114479
C	-1.570354	0.091727	1.748531
C	1.570354	-0.091727	1.748531
C	-1.160340	1.703247	-2.114479
C	1.801280	2.181340	-1.398088
C	-2.374692	3.901761	0.874197
C	0.361799	3.705806	2.283522
C	-0.275137	5.597910	-2.368696
C	2.038035	6.043952	-0.377904

C	-2.727666	7.738342	-0.241485
C	-0.957215	7.494610	2.272291
C	0.621962	9.569168	-2.104736
C	1.755244	9.815448	0.753234
C	-2.522693	11.560402	-1.327605
C	-2.171679	11.354506	1.728629
C	1.216543	13.537539	-1.360122
C	0.965803	13.649703	1.703128
C	-1.163673	14.980064	-0.065164
H	-0.604326	15.922252	-0.029439
H	-2.923900	3.891075	-0.141143
H	-0.019533	4.528594	2.946987
H	0.036760	2.768324	2.795423
H	-2.167851	1.642443	-1.777834
H	1.358270	-5.532107	-2.517828
H	3.304629	-6.874604	0.107376
H	-0.090102	-6.451159	-2.951105
H	-0.173131	-4.692444	-2.792596
H	3.233780	-8.640943	0.118606
H	2.771851	-7.748295	-1.335877
H	1.536749	-8.303455	2.731634
H	1.410246	-6.546649	2.582231
H	-0.054648	-7.531342	2.690107
H	-2.348580	-6.984853	-0.845017
H	-2.355064	-6.073056	0.670157
H	-2.588037	-5.233644	-0.869823
H	1.896673	-15.000534	0.748486
H	3.121504	-10.644019	-1.363563
H	2.718858	-3.049555	1.470796
H	2.038400	-11.678947	-2.302772
H	2.660857	-4.815255	1.407246
H	-1.538880	-9.947675	1.818827
H	2.923900	-3.891075	-0.141143
H	0.019533	-4.528594	2.946987
H	-0.036760	-2.768324	2.795423
H	-1.451753	-3.746383	2.182836
H	-1.072620	-10.510510	-2.438334
H	-2.340931	-10.680692	0.422463
H	2.794107	-12.238618	1.909177
H	3.211171	-12.402466	-1.194520
H	0.257244	-9.382856	-2.730857
H	-0.294305	-13.658651	2.568288
H	-1.544982	-14.580228	1.725021
H	-1.666438	-12.819047	1.835319
H	-1.345174	-8.769378	-2.299503

H	-1.960952	-12.738001	-1.281618
H	-1.758294	-14.490317	-1.387324
H	-0.704618	-13.421967	-2.321588
H	-2.389893	-8.928508	0.650818
H	1.717358	-14.958993	-1.009692
H	1.479854	-11.259812	2.572461
H	2.832245	-10.480598	1.739292
H	0.604326	-15.922252	-0.029439
H	0.054648	7.531342	2.690107
H	2.389893	8.928508	0.650818
H	-1.536749	8.303455	2.731634
H	-1.410246	6.546649	2.582231
H	2.340931	10.680692	0.422463
H	1.538880	9.947675	1.818827
H	1.072620	10.510510	-2.438334
H	1.345174	8.769378	-2.299503
H	-0.257244	9.382856	-2.730857
H	-3.233780	8.640943	0.118606
H	-2.771851	7.748295	-1.335877
H	-3.304629	6.874604	0.107376
H	1.666438	12.819047	1.835319
H	2.588037	5.233644	-0.869823
H	0.294305	13.658651	2.568288
H	2.348580	6.984853	-0.845017
H	-2.038400	11.678947	-2.302772
H	2.355064	6.073056	0.670157
H	0.090102	6.451159	-2.951105
H	0.173131	4.692444	-2.792596
H	-1.358270	5.532107	-2.517828
H	-2.794107	12.238618	1.909177
H	-3.211171	12.402466	-1.194520
H	1.758294	14.490317	-1.387324
H	1.544982	14.580228	1.725021
H	-1.479854	11.259812	2.572461
H	-2.832245	10.480598	1.739292
H	-3.121504	10.644019	-1.363563
H	0.704618	13.421967	-2.321588
H	1.960952	12.738001	-1.281618
H	2.440934	-0.054531	1.232257
H	-1.595803	1.018085	2.333097
H	0.946690	-0.788255	-2.677571
H	-1.610709	-0.745489	2.454276
H	2.167851	-1.642443	-1.777834
H	-2.074093	-1.359626	-2.069652
H	-1.861393	-3.111933	-1.973316

H	1.103246	-2.543562	-2.815692
H	-2.440934	0.054531	1.232257
H	1.610709	0.745489	2.454276
H	1.595803	-1.018085	2.333097
H	-2.558282	-2.231023	-0.608010
H	1.451753	3.746383	2.182836
H	-2.660857	4.815255	1.407246
H	1.861393	3.111933	-1.973316
H	-2.718858	3.049555	1.470796
H	2.558282	2.231023	-0.608010
H	-1.103246	2.543562	-2.815692
H	-0.946690	0.788255	-2.677571
H	2.074093	1.359626	-2.069652
H	-1.717358	14.958993	-1.009692
H	-1.896673	15.000534	0.748486

MP2/6311G optimized geometry, all-*deviant*-$Si_{15}Me_{32}$**

143
RI-MP2
Energy= -5608.88972518634364
TD B3LYP
Energy= -5620.80504223

Si	3.261618	-13.164370	0.646106
Si	3.113715	-11.232088	-0.694750
Si	1.825880	-9.551588	0.354969
Si	2.533726	-7.373526	-0.225765
Si	0.757799	-5.815224	-0.228528
Si	1.463321	-3.637742	0.357186
Si	0.179936	-1.956539	-0.695768
Si	0.000000	0.000000	0.616412
Si	-0.179936	1.956539	-0.695768
Si	-1.463321	3.637742	0.357186
Si	-0.757799	5.815224	-0.228528
Si	-2.533726	7.373526	-0.225765
Si	-1.825880	9.551588	0.354969
Si	-3.113715	11.232088	-0.694750
Si	-3.261618	13.164370	0.646106
C	1.553384	-13.794775	1.196341
C	4.084683	-14.563738	-0.337927
C	4.292821	-12.774047	2.193618
C	2.310831	-11.602369	-2.382686
C	4.916432	-10.689724	-1.009309
C	0.025776	-9.899934	-0.173844
C	1.900484	-9.662669	2.257011
C	3.298525	-7.297967	-1.971399
C	3.900512	-6.917252	1.023816
C	0.000000	-5.889071	-1.977164
C	-0.613883	-6.272781	1.015139
C	3.273979	-3.301237	-0.138906
C	1.359551	-3.548376	2.259543
C	1.021829	-1.631192	-2.375893
C	-1.608893	-2.518190	-1.045278
C	1.516712	0.263167	1.742505
C	-1.516712	-0.263167	1.742505
C	1.608893	2.518190	-1.045278
C	-1.021829	1.631192	-2.375893
C	-1.359551	3.548376	2.259543
C	-3.273979	3.301237	-0.138906
C	0.613883	6.272781	1.015139
C	0.000000	5.889071	-1.977164

C	-3.900512	6.917252	1.023816
C	-3.298525	7.297967	-1.971399
C	-1.900484	9.662669	2.257011
C	-0.025776	9.899934	-0.173844
C	-4.916432	10.689724	-1.009309
C	-2.310831	11.602369	-2.382686
C	-4.292821	12.774047	2.193618
C	-1.553384	13.794775	1.196341
C	-4.084683	14.563738	-0.337927
H	5.085949	-14.251764	-0.684937
H	4.194555	-15.460912	0.299910
H	3.470154	-14.828012	-1.217031
H	1.610916	-0.552919	2.479096
H	1.419098	1.212061	2.299451
H	2.452492	0.307575	1.159098
H	-1.610916	0.552919	2.479096
H	-1.419098	-1.212061	2.299451
H	-2.452492	-0.307575	1.159098
H	1.628672	3.362719	-1.755085
H	2.189597	1.689854	-1.488667
H	2.122461	2.835418	-0.121436
H	-0.422129	0.941230	-2.993774
H	-1.134248	2.576420	-2.936189
H	-2.026017	1.191524	-2.248268
H	2.026017	-1.191524	-2.248268
H	0.422129	-0.941230	-2.993774
H	1.134248	-2.576420	-2.936189
H	-2.189597	-1.689854	-1.488667
H	-2.122461	-2.835418	-0.121436
H	-1.628672	-3.362719	-1.755085
H	-0.316363	3.619573	2.612876
H	-1.784924	2.602616	2.636526
H	-1.928495	4.379726	2.712752
H	-3.549278	2.259306	0.103383
H	-3.432768	3.450684	-1.220753
H	-3.965152	3.968379	0.403937
H	3.965152	-3.968379	0.403937
H	3.549278	-2.259306	0.103383
H	3.432768	-3.450684	-1.220753
H	1.784924	-2.602616	2.636526
H	1.928495	-4.379726	2.712752
H	0.316363	-3.619573	2.612876
H	-0.707112	5.523526	-2.741679
H	0.217683	6.362978	2.041169
H	1.398398	5.495282	1.021749

H	0.916850	5.278202	-2.038938
H	0.268571	6.929436	-2.233459
H	1.090127	7.231241	0.746643
H	0.707112	-5.523526	-2.741679
H	-0.916850	-5.278202	-2.038938
H	-0.268571	-6.929436	-2.233459
H	-1.398398	-5.495282	1.021749
H	-0.217683	-6.362978	2.041169
H	-1.090127	-7.231241	0.746643
H	-4.377770	5.958495	0.757967
H	-3.568194	6.257396	-2.225794
H	-4.685145	7.694847	1.032821
H	-3.500182	6.828046	2.048522
H	-2.594407	7.662714	-2.738965
H	-4.215624	7.908781	-2.030119
H	3.500182	-6.828046	2.048522
H	2.594407	-7.662714	-2.738965
H	3.568194	-6.257396	-2.225794
H	4.377770	-5.958495	0.757967
H	4.685145	-7.694847	1.032821
H	4.215624	-7.908781	-2.030119
H	0.231367	10.959775	0.011347
H	0.124367	9.697885	-1.249889
H	0.684249	9.274994	0.395644
H	-1.515411	10.635941	2.612461
H	-1.279875	8.866570	2.709989
H	-2.932655	9.543760	2.632194
H	-0.684249	-9.274994	0.395644
H	1.279875	-8.866570	2.709989
H	-0.231367	-10.959775	0.011347
H	-0.124367	-9.697885	-1.249889
H	2.932655	-9.543760	2.632194
H	1.515411	-10.635941	2.612461
H	-2.897800	12.355526	-2.938892
H	-5.514591	11.540331	-1.386384
H	-5.393986	10.324104	-0.082179
H	-2.265530	10.685105	-2.998285
H	-4.966075	9.882958	-1.761372
H	-1.281431	11.985902	-2.267252
H	5.514591	-11.540331	-1.386384
H	5.393986	-10.324104	-0.082179
H	4.966075	-9.882958	-1.761372
H	2.897800	-12.355526	-2.938892
H	2.265530	-10.685105	-2.998285
H	1.281431	-11.985902	-2.267252

H	-3.820416	11.977516	2.795713
H	-5.309861	12.439480	1.922013
H	-4.387943	13.672896	2.831076
H	-1.651922	14.744646	1.749742
H	-3.470154	14.828012	-1.217031
H	-4.194555	15.460912	0.299910
H	-1.051302	13.070203	1.857654
H	-0.894392	13.975918	0.329039
H	-5.085949	14.251764	-0.684937
H	4.387943	-13.672896	2.831076
H	1.651922	-14.744646	1.749742
H	0.894392	-13.975918	0.329039
H	3.820416	-11.977516	2.795713
H	1.051302	-13.070203	1.857654
H	5.309861	-12.439480	1.922013

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{15}Me_{32}$**

143
RI-MP2
Energy= -5608.85418461303743
TD B3LYP
Energy= -5620.77305583

Si	0.000000	13.505616	-0.688330
Si	0.787672	11.614078	0.480448
Si	-0.616176	9.694480	0.326546
Si	0.364279	7.745728	-0.638145
Si	0.442387	5.807351	0.749710
Si	-0.710994	3.883133	-0.060625
Si	0.613010	1.930431	-0.412085
Si	0.000000	0.000000	0.847757
Si	-0.613010	-1.930431	-0.412085
Si	0.710994	-3.883133	-0.060625
Si	-0.442387	-5.807351	0.749710
Si	-0.364279	-7.745728	-0.638145
Si	0.616176	-9.694480	0.326546
Si	-0.787672	-11.614078	0.480448
Si	0.000000	-13.505616	-0.688330
C	-1.689778	14.129874	-0.085317
C	1.257434	14.907411	-0.446001
C	-0.099525	13.112340	-2.546905
C	2.576759	11.318634	-0.107612
C	0.916632	12.039026	2.336801
C	-1.306686	9.402124	2.079432
C	-2.144926	10.080170	-0.751623
C	2.161598	8.059250	-1.192049
C	-0.602541	7.422650	-2.249458
C	2.293335	5.451885	1.039753
C	-0.274973	6.149795	2.483087
C	-2.123732	3.565184	1.179769
C	-1.578388	4.227318	-1.723341
C	2.452480	2.243505	-0.018585
C	0.556564	1.596874	-2.288810
C	1.472303	-0.351148	2.007300
C	-1.472303	0.351148	2.007300
C	-0.556564	-1.596874	-2.288810
C	-2.452480	-2.243505	-0.018585
C	1.578388	-4.227318	-1.723341
C	2.123732	-3.565184	1.179769
C	0.274973	-6.149795	2.483087
C	-2.293335	-5.451885	1.039753

C	0.602541	-7.422650	-2.249458
C	-2.161598	-8.059250	-1.192049
C	1.306686	-9.402124	2.079432
C	2.144926	-10.080170	-0.751623
C	-0.916632	-12.039026	2.336801
C	-2.576759	-11.318634	-0.107612
C	0.099525	-13.112340	-2.546905
C	1.689778	-14.129874	-0.085317
C	-1.257434	-14.907411	-0.446001
H	2.248393	14.600232	-0.820987
H	0.937642	15.810276	-0.996212
H	1.345630	15.162754	0.624755
H	1.244560	-1.197627	2.679816
H	1.676775	0.535413	2.634112
H	-2.393240	0.592465	1.451294
H	-1.244560	1.197627	2.679816
H	-1.676775	-0.535413	2.634112
H	2.393240	-0.592465	1.451294
H	-2.618341	-2.472318	1.047262
H	-2.839876	-3.088149	-0.616256
H	-3.048464	-1.347751	-0.270200
H	0.464322	-1.377881	-2.643411
H	-1.203213	-0.740343	-2.551310
H	-0.924568	-2.481563	-2.839094
H	0.924568	2.481563	-2.839094
H	2.618341	2.472318	1.047262
H	2.839876	3.088149	-0.616256
H	3.048464	1.347751	-0.270200
H	-0.464322	1.377881	-2.643411
H	1.203213	0.740343	-2.551310
H	2.169514	-3.345217	-2.028508
H	1.747910	-3.330140	2.189235
H	2.755019	-2.723349	0.842944
H	2.765176	-4.461480	1.256639
H	0.860860	-4.449777	-2.530284
H	2.269550	-5.084362	-1.631464
H	-0.860860	4.449777	-2.530284
H	-2.269550	5.084362	-1.631464
H	-2.169514	3.345217	-2.028508
H	-1.747910	3.330140	2.189235
H	-2.755019	2.723349	0.842944
H	-2.765176	4.461480	1.256639
H	1.350000	-6.392860	2.449465
H	-2.422123	-4.601310	1.733032
H	-2.779436	-6.335209	1.491791

H	-0.253650	-6.992814	2.963275
H	0.148203	-5.259435	3.125008
H	-2.824765	-5.215062	0.103057
H	-0.148203	5.259435	3.125008
H	2.824765	5.215062	0.103057
H	2.422123	4.601310	1.733032
H	2.779436	6.335209	1.491791
H	-1.350000	6.392860	2.449465
H	0.253650	6.992814	2.963275
H	1.666635	-7.204179	-2.061125
H	-2.208675	-8.907804	-1.898026
H	-2.827458	-8.282305	-0.342120
H	0.167939	-6.568557	-2.799287
H	0.549220	-8.310941	-2.904259
H	-2.557220	-7.165789	-1.707700
H	2.827458	8.282305	-0.342120
H	-0.167939	6.568557	-2.799287
H	-0.549220	8.310941	-2.904259
H	2.208675	8.907804	-1.898026
H	2.557220	7.165789	-1.707700
H	-1.666635	7.204179	-2.061125
H	2.700817	-10.940835	-0.337602
H	1.868909	-10.318333	-1.793412
H	0.513293	-9.172902	2.811224
H	2.830238	-9.212645	-0.772177
H	2.029284	-8.566512	2.083009
H	1.835437	-10.310618	2.422946
H	-0.513293	9.172902	2.811224
H	-2.700817	10.940835	-0.337602
H	-1.868909	10.318333	-1.793412
H	-2.029284	8.566512	2.083009
H	-1.835437	10.310618	2.422946
H	-2.830238	9.212645	-0.772177
H	-1.583302	-12.907499	2.485292
H	-1.336605	-11.189071	2.903881
H	-2.630744	-11.093517	-1.186652
H	-3.042746	-10.480424	0.440323
H	-3.179320	-12.225994	0.082662
H	0.067539	-12.282721	2.773136
H	1.583302	12.907499	2.485292
H	-0.067539	12.282721	2.773136
H	2.630744	11.093517	-1.186652
H	1.336605	11.189071	2.903881
H	3.042746	10.480424	0.440323
H	3.179320	12.225994	0.082662

H	-0.937642	-15.810276	-0.996212
H	-0.876596	-12.776398	-2.939891
H	-1.345630	-15.162754	0.624755
H	1.978751	-15.030330	-0.655673
H	-2.248393	-14.600232	-0.820987
H	1.663578	-14.399495	0.984068
H	0.840435	-12.318243	-2.750450
H	2.478971	-13.370585	-0.227505
H	0.402431	-14.012857	-3.112844
H	-0.402431	14.012857	-3.112844
H	-0.840435	12.318243	-2.750450
H	-1.663578	14.399495	0.984068
H	-2.478971	13.370585	-0.227505
H	-1.978751	15.030330	-0.655673
H	0.876596	12.776398	-2.939891

MP2/6311G optimized geometry, all-*ortho*-$Si_{15}Me_{32}$**

143
RI-MP2
Energy= -5608.89675160802472
TD B3LYP
Energy= -5620.80519253

Si	1.231211	-11.994810	0.822771
Si	2.314671	-10.122013	-0.109082
Si	0.817196	-8.576921	-1.077437
Si	0.000000	-6.944801	0.418668
Si	1.370769	-5.034028	0.618412
Si	0.936551	-3.353115	-0.980354
Si	-0.758069	-1.832742	-0.358520
Si	0.000000	0.000000	0.920677
Si	0.758069	1.832742	-0.358520
Si	-0.936551	3.353115	-0.980354
Si	-1.370769	5.034028	0.618412
Si	0.000000	6.944801	0.418668
Si	-0.817196	8.576921	-1.077437
Si	-2.314671	10.122013	-0.109082
Si	-1.231211	11.994810	0.822771
C	-0.149392	-11.430812	1.987833
C	2.441210	-13.032896	1.838200
C	0.475372	-13.076575	-0.532998
C	3.481104	-10.731859	-1.481837
C	3.401277	-9.307870	1.218875
C	1.684373	-7.761136	-2.558216
C	-0.681069	-9.519524	-1.774239
C	-0.204600	-7.699425	2.151157
C	-1.736776	-6.437411	-0.163541
C	3.198887	-5.529750	0.461570
C	1.144126	-4.334332	2.370950
C	2.564610	-2.440426	-1.336204
C	0.402892	-4.172868	-2.611932
C	-2.097067	-2.731825	0.647231
C	-1.595338	-1.210805	-1.947525
C	1.422891	-0.547333	2.055638
C	-1.422891	0.547333	2.055638
C	2.097067	2.731825	0.647231
C	1.595338	1.210805	-1.947525
C	-2.564610	2.440426	-1.336204
C	-0.402892	4.172868	-2.611932
C	-1.144126	4.334332	2.370950
C	-3.198887	5.529750	0.461570

C	0.204600	7.699425	2.151157
C	1.736776	6.437411	-0.163541
C	-1.684373	7.761136	-2.558216
C	0.681069	9.519524	-1.774239
C	-3.401277	9.307870	1.218875
C	-3.481104	10.731859	-1.481837
C	-2.441210	13.032896	1.838200
C	-0.475372	13.076575	-0.532998
C	0.149392	11.430812	1.987833
H	3.307232	-13.356108	1.249385
H	-1.717074	-0.268836	2.724721
H	1.717074	0.268836	2.724721
H	-2.310114	0.842950	1.486253
H	1.128541	-1.398380	2.679171
H	-1.128541	1.398380	2.679171
H	2.310114	-0.842950	1.486253
H	2.396915	0.499325	-1.721675
H	2.038578	2.045955	-2.501090
H	2.491084	3.595567	0.100952
H	1.714789	3.091764	1.608073
H	0.885829	0.711828	-2.615758
H	2.936796	2.060059	0.856954
H	-2.936796	-2.060059	0.856954
H	-2.038578	-2.045955	-2.501090
H	-1.714789	-3.091764	1.608073
H	-2.396915	-0.499325	-1.721675
H	-2.491084	-3.595567	0.100952
H	-0.885829	-0.711828	-2.615758
H	-0.291787	3.424045	-3.404266
H	-2.975568	1.970265	-0.436725
H	-3.318050	3.138913	-1.717443
H	-1.146949	4.903609	-2.949199
H	-2.426772	1.656354	-2.087810
H	0.555391	4.694335	-2.513729
H	2.426772	-1.656354	-2.087810
H	3.318050	-3.138913	-1.717443
H	1.146949	-4.903609	-2.949199
H	-0.555391	-4.694335	-2.513729
H	2.975568	-1.970265	-0.436725
H	0.291787	-3.424045	-3.404266
H	-3.436084	5.908160	-0.538080
H	-3.848756	4.668276	0.651034
H	-1.438361	5.075559	3.122182
H	-0.103506	4.058251	2.570072
H	-1.760679	3.442246	2.525143

H	-3.462165	6.309779	1.184034
H	3.848756	-4.668276	0.651034
H	0.103506	-4.058251	2.570072
H	1.438361	-5.075559	3.122182
H	3.462165	-6.309779	1.184034
H	1.760679	-3.442246	2.525143
H	3.436084	-5.908160	-0.538080
H	1.724662	6.027244	-1.178698
H	-0.757233	7.985560	2.589244
H	2.171214	5.679169	0.496824
H	2.409929	7.301848	-0.164931
H	0.836713	8.593494	2.122730
H	0.675942	6.980737	2.830670
H	0.757233	-7.985560	2.589244
H	-0.675942	-6.980737	2.830670
H	-2.409929	-7.301848	-0.164931
H	-1.724662	-6.027244	-1.178698
H	-2.171214	-5.679169	0.496824
H	-0.836713	-8.593494	2.122730
H	0.365231	10.304802	-2.470615
H	1.346578	8.841307	-2.320129
H	1.270569	9.994023	-0.982269
H	-1.974628	8.518613	-3.295019
H	-2.592309	7.227681	-2.258083
H	-1.027367	7.043184	-3.059780
H	2.592309	-7.227681	-2.258083
H	-1.270569	-9.994023	-0.982269
H	1.027367	-7.043184	-3.059780
H	1.974628	-8.518613	-3.295019
H	-0.365231	-10.304802	-2.470615
H	-1.346578	-8.841307	-2.320129
H	-2.929782	11.184461	-2.312559
H	-4.182442	11.482617	-1.100082
H	-4.071446	9.903883	-1.889006
H	-4.134865	10.024171	1.605249
H	-2.811567	8.948735	2.067916
H	-3.952770	8.454950	0.811704
H	4.182442	-11.482617	-1.100082
H	4.071446	-9.903883	-1.889006
H	2.929782	-11.184461	-2.312559
H	4.134865	-10.024171	1.605249
H	2.811567	-8.948735	2.067916
H	3.952770	-8.454950	0.811704
H	0.924218	10.878237	1.446667
H	0.266234	12.524477	-1.117888

H	-0.230289	10.781488	2.781498
H	-1.936219	13.929874	2.209746
H	-2.799025	12.470842	2.692560
H	0.628838	12.290379	2.466385
H	-1.235285	13.446936	-1.225836
H	-3.307232	13.356108	1.249385
H	0.025658	13.946048	-0.095407
H	0.230289	-10.781488	2.781498
H	-0.628838	-12.290379	2.466385
H	-0.924218	-10.878237	1.446667
H	-0.025658	-13.946048	-0.095407
H	1.235285	-13.446936	-1.225836
H	-0.266234	-12.524477	-1.117888
H	2.799025	-12.470842	2.692560
H	1.936219	-13.929874	2.209746

MP2/6311G optimized geometry, all-*gauche*-$Si_{15}Me_{32}$**

143
RI-MP2
Energy= -5608.89074749154224
TD B3LYP
Energy= -5620.79327556

Si	2.094740	10.148389	-0.907253
Si	0.000000	9.077961	-0.805331
Si	-0.271781	7.594751	1.003666
Si	1.335249	5.907693	1.350942
Si	1.747919	4.349948	-0.367325
Si	-0.032064	3.029633	-1.165914
Si	-1.193529	1.642325	0.342626
Si	0.000000	0.000000	1.537315
Si	1.193529	-1.642325	0.342626
Si	0.032064	-3.029633	-1.165914
Si	-1.747919	-4.349948	-0.367325
Si	-1.335249	-5.907693	1.350942
Si	0.271781	-7.594751	1.003666
Si	0.000000	-9.077961	-0.805331
Si	-2.094740	-10.148389	-0.907253
C	1.849631	11.718989	-1.932204
C	3.277636	9.016886	-1.846297
C	2.741129	10.569300	0.815065
C	-1.300643	10.442702	-0.548807
C	-0.358258	8.232314	-2.468987
C	-0.273940	8.632611	2.597161
C	-2.004409	6.830731	0.833022
C	3.008661	6.722606	1.742990
C	0.800912	4.991404	2.929939
C	2.442315	5.268716	-1.881135
C	3.145751	3.227857	0.269255
C	-1.349333	4.162349	-1.941665
C	0.689268	1.987592	-2.583873
C	-2.058138	2.707062	1.661331
C	-2.574602	0.822457	-0.675845
C	1.276089	0.830987	2.677316
C	-1.276089	-0.830987	2.677316
C	2.574602	-0.822457	-0.675845
C	2.058138	-2.707062	1.661331
C	-0.689268	-1.987592	-2.583873
C	1.349333	-4.162349	-1.941665
C	-3.145751	-3.227857	0.269255
C	-2.442315	-5.268716	-1.881135

C	-0.800912	-4.991404	2.929939
C	-3.008661	-6.722606	1.742990
C	2.004409	-6.830731	0.833022
C	0.273940	-8.632611	2.597161
C	1.300643	-10.442702	-0.548807
C	0.358258	-8.232314	-2.468987
C	-3.277636	-9.016886	-1.846297
C	-2.741129	-10.569300	0.815065
C	-1.849631	-11.718989	-1.932204
H	1.312543	11.493671	-2.834540
H	2.803728	12.147004	-2.197793
H	1.300218	12.447362	-1.365982
H	1.562835	0.140742	3.476637
H	2.176110	1.092293	2.121364
H	0.857607	1.729291	3.136573
H	-0.857607	-1.729291	3.136573
H	-1.562835	-0.140742	3.476637
H	-2.176110	-1.092293	2.121364
H	2.176599	-0.412125	-1.603697
H	2.882785	-2.143418	2.108689
H	1.362995	-2.972544	2.457691
H	3.057291	-0.027109	-0.103278
H	2.468093	-3.617127	1.217095
H	3.334650	-1.566091	-0.935149
H	-2.176599	0.412125	-1.603697
H	-3.057291	0.027109	-0.103278
H	-3.334650	1.566091	-0.935149
H	-2.882785	2.143418	2.108689
H	-1.362995	2.972544	2.457691
H	-2.468093	3.617127	1.217095
H	-0.887428	-2.627438	-3.449389
H	-1.631066	-1.528505	-2.283857
H	0.881149	-4.978330	-2.498011
H	1.970458	-3.586890	-2.634975
H	0.014367	-1.209588	-2.889131
H	2.000380	-4.576842	-1.172131
H	1.631066	1.528505	-2.283857
H	-1.970458	3.586890	-2.634975
H	-2.000380	4.576842	-1.172131
H	-0.014367	1.209588	-2.889131
H	-0.881149	4.978330	-2.498011
H	0.887428	2.627438	-3.449389
H	-1.667421	-5.828093	-2.382910
H	-3.232781	-5.946962	-1.585373
H	-4.088409	-3.783603	0.284578

H	-3.272242	-2.360081	-0.382269
H	-2.937540	-2.892998	1.285146
H	-2.857488	-4.560412	-2.591579
H	4.088409	3.783603	0.284578
H	2.937540	2.892998	1.285146
H	3.232781	5.946962	-1.585373
H	2.857488	4.560412	-2.591579
H	3.272242	2.360081	-0.382269
H	1.667421	5.828093	-2.382910
H	-3.740743	-5.960463	2.025828
H	-3.392595	-7.263613	0.879061
H	-1.388160	-4.080267	3.065730
H	0.258270	-4.738918	2.887716
H	-0.959624	-5.633059	3.802191
H	-2.903397	-7.417499	2.579924
H	3.392595	7.263613	0.879061
H	2.903397	7.417499	2.579924
H	0.959624	5.633059	3.802191
H	1.388160	4.080267	3.065730
H	-0.258270	4.738918	2.887716
H	3.740743	5.960463	2.025828
H	0.516337	-8.000766	3.456384
H	-0.701569	-9.089557	2.769935
H	1.026253	-9.424092	2.534387
H	2.162383	-6.457355	-0.178273
H	2.765795	-7.590429	1.034447
H	2.138751	-6.014840	1.547019
H	-0.516337	8.000766	3.456384
H	0.701569	9.089557	2.769935
H	-2.138751	6.014840	1.547019
H	-2.162383	6.457355	-0.178273
H	-2.765795	7.590429	1.034447
H	-1.026253	9.424092	2.534387
H	2.302899	-10.007559	-0.515798
H	0.496657	-8.987034	-3.247367
H	1.123840	-10.980270	0.385622
H	1.269730	-7.635171	-2.407095
H	1.267875	-11.159183	-1.374216
H	-0.468040	-7.590670	-2.766030
H	-2.302899	10.007559	-0.515798
H	-1.123840	10.980270	0.385622
H	-1.267875	11.159183	-1.374216
H	0.468040	7.590670	-2.766030
H	-0.496657	8.987034	-3.247367
H	-1.269730	7.635171	-2.407095

H	-1.312543	-11.493671	-2.834540
H	-2.888978	-8.789197	-2.840766
H	-1.300218	-12.447362	-1.365982
H	-2.074393	-11.258117	1.323394
H	-2.803728	-12.147004	-2.197793
H	-3.719132	-11.037802	0.737517
H	-3.422126	-8.081686	-1.305791
H	-2.841651	-9.672033	1.424434
H	-4.251562	-9.499141	-1.960522
H	3.422126	8.081686	-1.305791
H	3.719132	11.037802	0.737517
H	2.888978	8.789197	-2.840766
H	2.841651	9.672033	1.424434
H	4.251562	9.499141	-1.960522
H	2.074393	11.258117	1.323394

MP2/6311G optimized geometry, all-*anti*-$Si_{16}Me_{34}$**

152
RI-MP2
Energy= -5977.51584961602657
TD B3LYP
Energy= -5990.21478779

H	1.174310	-10.773365	2.462000
H	1.174310	-10.773365	-2.462000
C	1.729449	-14.840756	1.537000
H	1.144523	-14.735345	-2.457000
Si	0.637537	-14.715988	0.000000
C	-0.550500	-16.189153	0.000000
C	1.729449	-14.840756	-1.537000
H	2.387658	-11.701219	1.574000
H	2.438900	-9.934254	-1.556000
H	2.387658	-11.701219	-1.574000
H	2.438900	-9.934254	1.556000
H	2.230764	-15.815109	-1.574000
H	-1.197497	-16.185698	0.884000
H	-1.197497	-16.185698	-0.884000
H	2.505992	-14.069302	-1.548000
H	0.002835	-17.135543	0.000000
H	2.505992	-14.069302	1.548000
H	1.144523	-14.735345	2.457000
H	2.230764	-15.815109	1.574000
Si	-0.658302	-8.824102	0.000000
H	-2.322780	-13.742906	-1.590000
H	-1.186051	-12.706705	2.462000
Si	0.658302	-10.785002	0.000000
H	-2.505545	-11.987777	1.532000
H	-2.322780	-13.742906	1.590000
H	-1.186051	-12.706705	-2.462000
H	-2.505545	-11.987777	-1.532000
C	1.767292	-10.798782	-1.542000
C	1.767292	-10.798782	1.542000
Si	-0.657077	-12.744077	0.000000
C	-1.770115	-12.798295	-1.540000
C	-1.770115	-12.798295	1.540000
Si	0.658320	-6.863176	0.000000
H	-2.387658	-9.740319	-1.574000
H	-1.174310	-8.812465	-2.462000
Si	-0.658284	-4.902276	0.000000
H	-2.438882	-4.051528	1.556000
C	1.767310	-6.849396	1.542000

C	-1.767274	-4.916056	1.542000
H	2.438918	-7.713924	-1.556000
H	-2.438900	-7.973354	-1.556000
H	2.387676	-5.946959	1.574000
H	1.174328	-6.874813	2.462000
C	-1.767292	-8.837882	1.542000
C	-1.767274	-4.916056	-1.542000
H	-1.174310	-8.812465	2.462000
H	-2.387640	-5.818493	1.574000
H	-2.387640	-5.818493	-1.574000
H	-2.438882	-4.051528	-1.556000
Si	0.658320	-2.941376	0.000000
H	1.174328	-6.874813	-2.462000
H	-2.438900	-7.973354	1.556000
H	-2.387658	-9.740319	1.574000
H	-1.174292	-4.890639	-2.462000
C	-1.767292	-8.837882	-1.542000
C	1.767310	-6.849396	-1.542000
H	-1.174292	-4.890639	2.462000
H	2.438918	-7.713924	1.556000
H	2.387676	-5.946959	-1.574000
H	-1.174310	10.773365	2.462000
H	-1.174310	10.773365	-2.462000
C	-1.729449	14.840756	1.537000
H	-1.144523	14.735345	-2.457000
Si	-0.637537	14.715988	0.000000
C	0.550500	16.189153	0.000000
C	-1.729449	14.840756	-1.537000
H	-2.387658	11.701219	1.574000
H	-2.438900	9.934254	-1.556000
H	-2.387658	11.701219	-1.574000
H	-2.438900	9.934254	1.556000
H	-2.230764	15.815109	-1.574000
H	1.197497	16.185698	0.884000
H	1.197497	16.185698	-0.884000
H	-2.505992	14.069302	-1.548000
H	-0.002835	17.135543	0.000000
H	-2.505992	14.069302	1.548000
H	-1.144523	14.735345	2.457000
H	-2.230764	15.815109	1.574000
Si	0.658302	8.824102	0.000000
H	2.322780	13.742906	-1.590000
H	1.186051	12.706705	2.462000
Si	-0.658302	10.785002	0.000000
H	2.505545	11.987777	1.532000

H	2.322780	13.742906	1.590000
H	1.186051	12.706705	-2.462000
H	2.505545	11.987777	-1.532000
C	-1.767292	10.798782	-1.542000
C	-1.767292	10.798782	1.542000
Si	0.657077	12.744077	0.000000
C	1.770115	12.798295	-1.540000
C	1.770115	12.798295	1.540000
Si	-0.658320	6.863176	0.000000
H	2.387658	9.740319	-1.574000
H	1.174310	8.812465	-2.462000
Si	0.658284	4.902276	0.000000
H	2.438882	4.051528	1.556000
C	-1.767310	6.849396	1.542000
C	1.767274	4.916056	1.542000
H	-2.438918	7.713924	-1.556000
H	2.438900	7.973354	-1.556000
H	-2.387676	5.946959	1.574000
H	-1.174328	6.874813	2.462000
C	1.767292	8.837882	1.542000
C	1.767274	4.916056	-1.542000
H	1.174310	8.812465	2.462000
H	2.387640	5.818493	1.574000
H	2.387640	5.818493	-1.574000
H	2.438882	4.051528	-1.556000
Si	-0.658320	2.941376	0.000000
H	-1.174328	6.874813	-2.462000
H	2.438900	7.973354	1.556000
H	2.387658	9.740319	1.574000
H	1.174292	4.890639	-2.462000
C	1.767292	8.837882	-1.542000
C	-1.767310	6.849396	-1.542000
H	1.174292	4.890639	2.462000
H	-2.438918	7.713924	1.556000
H	-2.387676	5.946959	-1.574000
H	1.174328	-2.929739	2.462000
C	-1.767292	-0.966670	-1.542000
H	1.174328	-2.929739	-2.462000
C	-1.767292	-0.966670	1.542000
Si	-0.658302	-0.980450	0.000000
H	2.438918	-2.090629	-1.556000
H	2.387676	-3.857593	-1.574000
H	2.387676	-3.857593	1.574000
H	-2.438900	-1.831198	1.556000
H	2.438918	-2.090629	1.556000

H	-1.174310	-0.992087	-2.462000
H	-2.438900	-1.831198	-1.556000
C	1.767310	-2.955156	-1.542000
H	-2.387658	-0.064233	-1.574000
H	-1.174310	-0.992087	2.462000
C	1.767310	-2.955156	1.542000
H	-2.387658	-0.064233	1.574000
Si	0.658302	0.980450	0.000000
H	-1.174328	2.929739	2.462000
C	1.767292	0.966670	-1.542000
H	-1.174328	2.929739	-2.462000
C	1.767292	0.966670	1.542000
H	-2.438918	2.090629	-1.556000
H	-2.387676	3.857593	-1.574000
H	-2.387676	3.857593	1.574000
H	2.438900	1.831198	1.556000
H	-2.438918	2.090629	1.556000
H	1.174310	0.992087	-2.462000
H	2.438900	1.831198	-1.556000
C	-1.767310	2.955156	-1.542000
H	2.387658	0.064233	-1.574000
H	1.174310	0.992087	2.462000
C	-1.767310	2.955156	1.542000
H	2.387658	0.064233	1.574000

MP2/6311G optimized geometry, all-*transoid*-$Si_{16}Me_{34}$**

152
RI-MP2
Energy= -5977.53175378015749
TD B3LYP
Energy=-5990.21645571

Si	0.131280	14.445624	-0.588247
Si	-0.049262	12.511034	0.739835
Si	-0.204365	10.585082	-0.604036
Si	0.282630	8.662285	0.661410
Si	-0.478256	6.734597	-0.452474
Si	0.542012	4.813888	0.445079
Si	-0.648579	2.884517	-0.183953
Si	0.672839	0.964990	0.139980
Si	-0.672839	-0.964990	0.139980
Si	0.648579	-2.884517	-0.183953
Si	-0.542012	-4.813888	0.445079
Si	0.478256	-6.734597	-0.452474
Si	-0.282630	-8.662285	0.661410
Si	0.204365	-10.585082	-0.604036
Si	0.049262	-12.511034	0.739835
Si	-0.131280	-14.445624	-0.588247
C	-1.140648	14.421046	-1.986535
C	-0.169315	15.983254	0.470952
C	1.862480	14.557124	-1.337183
C	1.465016	12.418275	1.884574
C	-1.610200	12.629337	1.816269
C	1.015518	10.685215	-2.056907
C	-1.968269	10.483678	-1.302342
C	2.154744	8.505709	0.943622
C	-0.571181	8.826087	2.350626
C	-2.359669	6.560074	-0.254728
C	-0.078183	6.900078	-2.302213
C	2.330831	4.656987	-0.174990
C	0.571181	4.981153	2.337286
C	-1.131141	3.049776	-2.014008
C	-2.235695	2.714385	0.846141
C	1.950843	0.802848	-1.256334
C	1.599168	1.132532	1.790076
C	-1.950843	-0.802848	-1.256334
C	-1.599168	-1.132532	1.790076
C	1.131141	-3.049776	-2.014008
C	2.235695	-2.714385	0.846141
C	-2.330831	-4.656987	-0.174990

C	-0.571181	-4.981153	2.337286
C	0.078183	-6.900078	-2.302213
C	2.359669	-6.560074	-0.254728
C	-2.154744	-8.505709	0.943622
C	0.571181	-8.826087	2.350626
C	-1.015518	-10.685215	-2.056907
C	1.968269	-10.483678	-1.302342
C	-1.465016	-12.418275	1.884574
C	1.610200	-12.629337	1.816269
C	0.169315	-15.983254	0.470952
C	-1.862480	-14.557124	-1.337183
C	1.140648	-14.421046	-1.986535
H	0.247417	-3.065407	-2.660949
H	2.920859	-3.548198	0.655366
H	2.767890	-1.787877	0.604725
H	-1.469122	-0.788793	-2.239946
H	-2.651468	6.546764	0.800934
H	-0.304335	7.992957	3.010414
H	-2.886134	7.392188	-0.735411
H	-2.722728	5.632139	-0.710391
H	-0.279053	9.753745	2.855223
H	-1.661719	8.833980	2.248604
H	2.535244	9.343697	1.538669
H	2.399243	7.582245	1.479685
H	2.703307	8.494504	-0.004397
H	-0.497400	7.822857	-2.717742
H	1.002766	6.917669	-2.478354
H	-0.494896	6.061947	-2.872278
H	0.539860	16.042687	1.303582
H	-1.727808	11.743214	2.449182
H	1.114511	4.149105	2.798940
H	-2.512110	12.720297	1.201592
H	1.063966	5.909595	2.646573
H	2.043301	10.831967	-1.707747
H	-0.441806	4.989350	2.753860
H	2.943947	5.495888	0.173468
H	2.796905	3.734391	0.187671
H	2.375862	4.643808	-1.269331
H	-2.236549	11.400557	-1.838872
H	0.767765	11.519493	-2.723004
H	1.563698	13.332465	2.481388
H	-1.567444	13.504579	2.474227
H	-2.706081	10.338192	-0.505967
H	2.630844	14.602239	-0.558034
H	1.963578	15.458279	-1.953221

H	2.084295	13.693703	-1.972521
H	-2.067436	9.648723	-2.004944
H	-0.966149	13.586357	-2.673858
H	-1.093120	15.346070	-2.573129
H	-2.161878	14.326958	-1.601728
H	0.995892	9.767903	-2.655308
H	-1.179048	15.985661	0.894717
H	2.392976	12.293097	1.316364
H	1.385532	11.577775	2.582728
H	-0.057109	16.897082	-0.124189
H	2.651468	-6.546764	0.800934
H	0.304335	-7.992957	3.010414
H	2.886134	-7.392188	-0.735411
H	2.722728	-5.632139	-0.710391
H	0.279053	-9.753745	2.855223
H	1.661719	-8.833980	2.248604
H	-2.535244	-9.343697	1.538669
H	-2.399243	-7.582245	1.479685
H	-2.703307	-8.494504	-0.004397
H	0.497400	-7.822857	-2.717742
H	-1.002766	-6.917669	-2.478354
H	0.494896	-6.061947	-2.872278
H	-0.539860	-16.042687	1.303582
H	1.727808	-11.743214	2.449182
H	-1.114511	-4.149105	2.798940
H	2.512110	-12.720297	1.201592
H	-1.063966	-5.909595	2.646573
H	-2.043301	-10.831967	-1.707747
H	0.441806	-4.989350	2.753860
H	-2.943947	-5.495888	0.173468
H	-2.796905	-3.734391	0.187671
H	-2.375862	-4.643808	-1.269331
H	2.236549	-11.400557	-1.838872
H	-0.767765	-11.519493	-2.723004
H	-1.563698	-13.332465	2.481388
H	1.567444	-13.504579	2.474227
H	2.706081	-10.338192	-0.505967
H	-2.630844	-14.602239	-0.558034
H	-1.963578	-15.458279	-1.953221
H	-2.084295	-13.693703	-1.972521
H	2.067436	-9.648723	-2.004944
H	0.966149	13.586357	-2.673858
H	1.093120	-15.346070	-2.573129
H	2.161878	-14.326958	-1.601728
H	-0.995892	-9.767903	-2.655308

H	1.179048	-15.985661	0.894717
H	-2.392976	-12.293097	1.316364
H	-1.385532	-11.577775	2.582728
H	0.057109	-16.897082	-0.124189
H	0.906942	1.143175	2.638895
H	2.531121	-0.121390	-1.158540
H	-2.767890	1.787877	0.604725
H	2.657943	1.639797	-1.243620
H	-2.017355	2.701885	1.919433
H	-1.762741	2.213124	-2.332961
H	-1.690792	3.974095	-2.195471
H	-2.920859	3.548198	0.655366
H	1.469122	0.788793	-2.239946
H	2.294863	0.298761	1.938133
H	2.182175	2.059240	1.825398
H	-0.247417	3.065407	-2.660949
H	2.017355	-2.701885	1.919433
H	1.690792	-3.974095	-2.195471
H	-2.182175	-2.059240	1.825398
H	1.762741	-2.213124	-2.332961
H	-0.906942	-1.143175	2.638895
H	-2.657943	-1.639797	-1.243620
H	-2.531121	0.121390	-1.158540
H	-2.294863	-0.298761	1.938133

MP2/6311G optimized geometry, all-*deviant*-$Si_{16}Me_{34}$**

152
RI-MP2
Energy= -5977.50908169800277
TD B3LYP
Energy= -5990.19879798

H	-2.536136	-6.505409	1.275256
H	2.467737	-13.545627	-1.441678
H	-2.886963	-13.686908	0.833667
Si	-0.085564	-6.796117	0.708708
H	0.579536	-11.556745	2.805508
C	-1.605050	-6.651462	1.851476
C	-2.271975	-8.836935	-0.982419
H	1.283742	-14.354706	-2.509682
H	0.091540	-7.864205	-2.922381
H	2.364207	-7.156674	1.227435
H	-2.611195	-7.910000	-1.482263
H	-2.004133	-13.491746	-2.184869
H	0.437606	-9.612927	-2.806237
H	1.642718	-5.949205	2.330163
H	-0.766531	-12.286953	-2.645299
H	-0.726195	-10.342046	2.686715
H	-2.936057	-11.912484	1.050463
H	0.982788	-9.817297	2.750841
H	-1.496050	-5.801651	2.549923
H	-1.718353	-7.572796	2.453496
H	2.437907	-15.330491	-1.555712
C	1.462578	-6.913108	1.818186
C	-0.486619	-16.080684	-0.332644
C	1.509636	-14.663704	1.531095
H	-2.335302	-11.750130	-1.977568
Si	-0.405969	-8.734183	-0.604073
H	1.591084	-8.428664	-2.126864
C	0.517648	-8.647785	-2.271658
H	1.339038	-7.689885	2.593016
H	-2.868354	-8.964082	-0.061307
H	-2.493659	-9.685351	-1.655423
Si	0.240235	-4.858085	-0.602871
H	-1.916099	-12.915592	2.123739
Si	0.405969	-10.686296	0.450613
C	2.248643	-10.834950	-0.016442
C	0.298486	-10.587134	2.353239
Si	-0.828958	-12.613835	-0.137822
C	1.804849	-14.423365	-1.537498

H	2.132573	-15.577935	1.539528
H	-1.205105	-16.203454	0.497947
Si	0.563722	-14.515115	-0.106804
C	-2.276850	-12.799847	1.086068
C	-1.550483	-12.523134	-1.902959
H	0.157975	-16.979526	-0.360824
H	2.176401	-13.797403	1.692362
H	0.813615	-14.720678	2.387898
H	2.720031	-11.691942	0.498576
H	2.792657	-9.918945	0.282065
H	2.383811	-10.971152	-1.104312
H	-1.059949	-16.045051	-1.276728
H	2.536136	6.505409	1.275256
H	-2.467737	13.545627	-1.441678
H	2.886963	13.686908	0.833667
Si	0.085564	6.796117	0.708708
H	-0.579536	11.556745	2.805508
C	1.605050	6.651462	1.851476
C	2.271975	8.836935	-0.982419
H	-1.283742	14.354706	-2.509682
H	-0.091540	7.864205	-2.922381
H	-2.364207	7.156674	1.227435
H	2.611195	7.910000	-1.482263
H	2.004133	13.491746	-2.184869
H	-0.437606	9.612927	-2.806237
H	-1.642718	5.949205	2.330163
H	0.766531	12.286953	-2.645299
H	0.726195	10.342046	2.686715
H	2.936057	11.912484	1.050463
H	-0.982788	9.817297	2.750841
H	1.496050	5.801651	2.549923
H	1.718353	7.572796	2.453496
H	-2.437907	15.330491	-1.555712
C	-1.462578	6.913108	1.818186
C	0.486619	16.080684	-0.332644
C	-1.509636	14.663704	1.531095
H	2.335302	11.750130	-1.977568
Si	0.405969	8.734183	-0.604073
H	-1.591084	8.428664	-2.126864
C	-0.517648	8.647785	-2.271658
H	-1.339038	7.689885	2.593016
H	2.868354	8.964082	-0.061307
H	2.493659	9.685351	-1.655423
Si	-0.240235	4.858085	-0.602871
H	1.916099	12.915592	2.123739

Si	-0.405969	10.686296	0.450613
C	-2.248643	10.834950	-0.016442
C	-0.298486	10.587134	2.353239
Si	0.828958	12.613835	-0.137822
C	-1.804849	14.423365	-1.537498
H	-2.132573	15.577935	1.539528
H	1.205105	16.203454	0.497947
Si	-0.563722	14.515115	-0.106804
C	2.276850	12.799847	1.086068
C	1.550483	12.523134	-1.902959
H	-0.157975	16.979526	-0.360824
H	-2.176401	13.797403	1.692362
H	-0.813615	14.720678	2.387898
H	-2.720031	11.691942	0.498576
H	-2.792657	9.918945	0.282065
H	-2.383811	10.971152	-1.104312
H	1.059949	16.045051	-1.276728
Si	0.576009	2.905951	0.448351
C	2.416749	2.757319	-0.026274
C	0.476340	3.005014	2.351408
H	-2.678103	4.558022	0.003112
C	-2.119852	4.783519	-0.923577
H	1.162270	3.774830	2.746236
C	0.629993	4.973163	-2.295545
H	-2.365646	4.008256	-1.670275
H	-2.482910	5.754146	-1.310557
H	0.759244	2.035380	2.802468
H	-0.546962	3.250086	2.689101
Si	-0.660844	0.979195	-0.134881
H	2.890247	1.900299	0.486759
H	2.961986	3.673308	0.270044
H	2.547449	2.621173	-1.114697
H	0.447118	4.052689	-2.881556
H	1.722427	5.094170	-2.184963
H	0.246727	5.829066	-2.880715
Si	0.660844	-0.979195	-0.134881
C	1.438928	-1.114674	-1.870368
C	2.085428	-0.898997	1.132203
H	-1.711303	0.661960	2.144670
C	-2.085428	0.898997	1.132203
H	2.825721	-0.129854	0.850440
C	-1.438928	1.114674	-1.870368
H	-2.825721	0.129854	0.850440
H	-2.609880	1.871621	1.183516
H	2.609880	-1.871621	1.183516

H	1.711303	-0.661960	2.144670
Si	-0.576009	-2.905951	0.448351
H	2.131327	-1.974403	-1.928132
H	2.015103	-0.199068	-2.102342
H	0.669811	-1.239683	-2.653384
H	-2.015103	0.199068	-2.102342
H	-0.669811	1.239683	-2.653384
H	-2.131327	1.974403	-1.928132
C	-2.416749	-2.757319	-0.026274
C	-0.476340	-3.005014	2.351408
H	2.678103	-4.558022	0.003112
C	2.119852	-4.783519	-0.923577
H	-1.162270	-3.774830	2.746236
C	-0.629993	-4.973163	-2.295545
H	2.365646	-4.008256	-1.670275
H	2.482910	-5.754146	-1.310557
H	-0.759244	-2.035380	2.802468
H	0.546962	-3.250086	2.689101
H	-2.890247	-1.900299	0.486759
H	-2.961986	-3.673308	0.270044
H	-2.547449	-2.621173	-1.114697
H	-0.447118	-4.052689	-2.881556
H	-1.722427	-5.094170	-2.184963
H	-0.246727	-5.829066	-2.880715

MP2/6311G optimized geometry, all-*eclipsed*-$Si_{16}Me_{34}$**

152
RI-MP2
Energy= -5977.47069223304152
TD B3LYP
Energy= -5990.16455308

Si	-2.422002	14.255305	-0.114916
Si	-0.781773	12.581297	-0.390122
Si	-1.284653	10.578058	0.794437
Si	-1.511275	8.602593	-0.523076
Si	-0.002164	6.823916	-0.024730
Si	-0.990181	4.762146	0.655404
Si	-0.520179	2.865682	-0.712801
Si	0.582208	1.040864	0.356984
Si	-0.582208	-1.040864	0.356984
Si	0.520179	-2.865682	-0.712801
Si	0.990181	-4.762146	0.655404
Si	0.002164	-6.823916	-0.024730
Si	1.511275	-8.602593	-0.523076
Si	1.284653	-10.578058	0.794437
Si	0.781773	-12.581297	-0.390122
Si	2.422002	-14.255305	-0.114916
C	-4.111139	13.692675	-0.768448
C	-1.882447	15.773097	-1.121231
C	-2.595126	14.790669	1.696069
C	0.863923	13.255653	0.305602
C	-0.520179	12.359915	-2.265506
C	0.036261	10.425590	2.160760
C	-2.942830	10.760548	1.724730
C	-3.344282	8.092618	-0.400958
C	-1.229530	9.004976	-2.368884
C	1.270793	7.270409	1.322535
C	1.025570	6.569967	-1.614564
C	-2.893891	4.916801	0.671722
C	-0.497069	4.515842	2.480527
C	-2.211637	2.303505	-1.399259
C	0.524320	3.286279	-2.251313
C	0.895840	1.446861	2.196848
C	2.315566	0.935145	-0.429904
C	-0.895840	-1.446861	2.196848
C	-2.315566	-0.935145	-0.429904
C	2.211637	-2.303505	-1.399259
C	-0.524320	-3.286279	-2.251313
C	0.497069	-4.515842	2.480527

C	2.893891	-4.916801	0.671722
C	-1.270793	-7.270409	1.322535
C	-1.025570	-6.569967	-1.614564
C	3.344282	-8.092618	-0.400958
C	1.229530	-9.004976	-2.368884
C	-0.036261	-10.425590	2.160760
C	2.942830	-10.760548	1.724730
C	0.520179	-12.359915	-2.265506
C	-0.863923	-13.255653	0.305602
C	1.882447	-15.773097	-1.121231
C	2.595126	-14.790669	1.696069
C	4.111139	-13.692675	-0.768448
H	-2.836654	-1.902345	-0.303672
H	0.044676	-1.583117	2.758183
H	-1.489961	-2.373893	2.290702
H	1.489961	2.373893	2.290702
H	1.463838	0.630292	2.679831
H	-3.642045	7.837372	0.630413
H	-2.905243	11.624496	2.412737
H	0.800450	7.438589	2.306421
H	1.799721	5.798032	-1.453372
H	-1.936883	9.784482	-2.705332
H	1.537123	7.508905	-1.896319
H	1.144018	14.191082	-0.213744
H	1.684183	12.528637	0.159521
H	-0.204200	9.364066	-2.563785
H	1.829685	8.183029	1.048355
H	1.998762	6.444793	1.429127
H	-3.553222	7.219666	-1.044937
H	-3.982408	8.928418	-0.743268
H	-3.791962	10.907162	1.035009
H	1.055193	10.319593	1.750781
H	-3.147614	9.856383	2.327414
H	-0.166244	9.553369	2.807778
H	-2.616756	16.592666	-1.005615
H	-4.042504	13.380341	-1.826481
H	-1.397332	8.105002	-2.989019
H	0.399757	6.256163	-2.467863
H	-0.899224	16.149180	-0.784920
H	0.016212	11.331452	2.794758
H	-3.309147	15.631725	1.777532
H	-1.806769	15.534887	-2.197534
H	-1.625255	15.129691	2.103242
H	-4.510591	12.844027	-0.185734
H	-2.965495	13.968629	2.333417

H	-4.841172	14.521607	-0.707273
H	-1.439241	12.025397	-2.777180
H	0.274925	11.623049	-2.477937
H	-0.214664	13.326575	-2.707493
H	0.792433	13.472376	1.386261
H	3.642045	-7.837372	0.630413
H	2.905243	-11.624496	2.412737
H	-0.800450	-7.438589	2.306421
H	-1.799721	-5.798032	-1.453372
H	1.936883	-9.784482	-2.705332
H	-1.537123	-7.508905	-1.896319
H	-1.144018	-14.191082	-0.213744
H	-1.684183	-12.528637	0.159521
H	0.204200	-9.364066	-2.563785
H	-1.829685	-8.183029	1.048355
H	-1.998762	-6.444793	1.429127
H	3.553222	-7.219666	-1.044937
H	3.982408	-8.928418	-0.743268
H	3.791962	-10.907162	1.035009
H	-1.055193	-10.319593	1.750781
H	3.147614	-9.856383	2.327414
H	0.166244	-9.553369	2.807778
H	2.616756	-16.592666	-1.005615
H	4.042504	-13.380341	-1.826481
H	1.397332	-8.105002	-2.989019
H	-0.399757	-6.256163	-2.467863
H	0.899224	-16.149180	-0.784920
H	-0.016212	-11.331452	2.794758
H	3.309147	-15.631725	1.777532
H	1.806769	-15.534887	-2.197534
H	1.625255	-15.129691	2.103242
H	4.510591	-12.844027	-0.185734
H	2.965495	-13.968629	2.333417
H	4.841172	-14.521607	-0.707273
H	1.439241	-12.025397	-2.777180
H	-0.274925	-11.623049	-2.477937
H	0.214664	-13.326575	-2.707493
H	-0.792433	-13.472376	1.386261
H	1.541952	3.623124	-1.989586
H	-3.352671	3.983844	1.048274
H	0.042303	4.080908	-2.848500
H	0.616031	2.388541	-2.890531
H	0.594132	4.418037	2.611885
H	-2.899225	1.982699	-0.597674
H	-0.975843	3.612303	2.898622

H	-0.835441	5.385619	3.073766
H	-3.303174	5.113274	-0.334320
H	-3.207521	5.740936	1.337764
H	-2.081402	1.458581	-2.099486
H	-2.696626	3.129484	-1.951730
H	-1.541952	-3.623124	-1.989586
H	3.352671	-3.983844	1.048274
H	-0.042303	-4.080908	-2.848500
H	-0.616031	-2.388541	-2.890531
H	-0.594132	-4.418037	2.611885
H	2.899225	-1.982699	-0.597674
H	0.975843	-3.612303	2.898622
H	0.835441	-5.385619	3.073766
H	3.303174	-5.113274	-0.334320
H	3.207521	-5.740936	1.337764
H	2.081402	-1.458581	-2.099486
H	2.696626	-3.129484	-1.951730
H	2.274483	0.708994	-1.509120
H	-1.463838	-0.630292	2.679831
H	2.923601	0.154799	0.061791
H	2.836654	1.902345	-0.303672
H	-2.274483	-0.708994	-1.509120
H	-0.044676	1.583117	2.758183
H	-2.923601	-0.154799	0.061791

MP2/6311G optimized geometry, all-*ortho*-$Si_{16}Me_{34}$**

152
RI-MP2
Energy= -5977.51832167021712
TD B3LYP
Energy= -5990.20131302

H	-6.150617	10.246156	1.019151
Si	-2.367695	9.192236	0.880127
C	-3.004752	9.768336	2.577509
C	-0.476328	9.075411	1.019047
Si	-2.885644	10.834073	-0.732622
H	-1.346624	12.552024	0.286155
H	-4.374849	12.576323	2.125155
H	-6.526141	10.145286	-0.705801
Si	-4.882934	11.990799	-0.261001
C	-1.478947	12.114950	-0.709381
C	-2.961688	10.115168	-2.488747
H	-6.229113	13.648703	-1.563628
H	-5.549751	12.421594	-2.640599
H	-7.247808	11.420639	0.284067
H	-2.610964	10.758992	2.832243
H	-2.690699	9.074773	3.365683
H	-4.098193	9.827157	2.605891
Si	-3.308940	7.071655	0.447387
H	-1.679703	12.935838	-1.407499
H	-0.526563	11.658304	-1.000288
C	-6.332585	10.840346	0.117485
C	-4.619690	13.137449	1.217814
C	-5.337136	13.044085	-1.765122
H	-0.055159	10.042613	1.315757
H	-0.012690	8.791119	0.068667
H	-0.175941	8.337025	1.769537
H	-3.804861	13.845654	1.034018
H	-4.527647	13.730855	-2.035111
H	-5.524950	13.721057	1.421954
H	-3.151130	10.909022	-3.220156
H	-3.757513	9.370660	-2.594085
H	-2.016117	9.634180	-2.759649
H	-2.732904	6.087912	2.698129
C	-4.995922	7.303897	-0.400548
C	-3.648775	6.224095	2.113631
H	-0.362366	7.396795	-1.827910
H	1.072065	4.870190	2.195517
C	0.248607	5.396919	1.700187

H	-4.896042	7.753539	-1.394392
H	-4.104133	5.238197	1.974580
C	1.106314	4.156822	-0.950921
H	0.828208	3.629603	-1.869453
C	-3.175600	4.518302	-1.868727
H	-4.337803	6.827700	2.715131
H	-0.572653	6.062522	-2.967544
H	-3.875015	5.085656	-2.493071
H	1.530075	5.124873	-1.241101
H	0.621900	6.380862	1.393814
H	1.898239	3.579418	-0.462924
H	-3.768872	3.907071	-1.180030
Si	-0.381852	4.405698	0.203911
H	-0.537503	5.556392	2.446161
H	-2.622277	3.837832	-2.526109
H	-5.651416	7.950905	0.193644
H	-1.806362	7.324504	-2.845485
Si	-1.176791	2.333033	1.005287
H	-5.504402	6.340948	-0.523248
C	-1.101474	6.718595	-2.266962
Si	-1.995895	5.689405	-0.943711
H	6.150617	-10.246156	1.01915
Si	2.367695	-9.192236	0.880127
C	3.004752	-9.768336	2.577509
C	0.476328	-9.075411	1.019047
Si	2.885644	-10.834073	-0.732622
H	1.346624	-12.552024	0.286155
H	4.374849	-12.576323	2.125155
H	6.526141	-10.145286	-0.705801
Si	4.882934	-11.990799	-0.261001
C	1.478947	-12.114950	-0.709381
C	2.961688	-10.115168	-2.488747
H	6.229113	-13.648703	-1.563628
H	5.549751	-12.421594	-2.640599
H	7.247808	-11.420639	0.284067
H	2.610964	-10.758992	2.832243
H	2.690699	-9.074773	3.365683
H	4.098193	-9.827157	2.605891
Si	3.308940	-7.071655	0.447387
H	1.679703	-12.935838	-1.407499
H	0.526563	-11.658304	-1.000288
C	6.332585	-10.840346	0.117485
C	4.619690	-13.137449	1.217814
C	5.337136	-13.044085	-1.765122
H	0.055159	-10.042613	1.315757

H	0.012690	-8.791119	0.068667
H	0.175941	-8.337025	1.769537
H	3.804861	-13.845654	1.034018
H	4.527647	-13.730855	-2.035111
H	5.524950	-13.721057	1.421954
H	3.151130	-10.909022	-3.220156
H	3.757513	-9.370660	-2.594085
H	2.016117	-9.634180	-2.759649
H	2.732904	-6.087912	2.698129
C	4.995922	-7.303897	-0.400548
C	3.648775	-6.224095	2.113631
H	0.362366	-7.396795	-1.827910
H	-1.072065	-4.870190	2.195517
C	-0.248607	-5.396919	1.700187
H	4.896042	-7.753539	-1.394392
H	4.104133	-5.238197	1.974580
C	-1.106314	-4.156822	-0.950921
H	-0.828208	-3.629603	-1.869453
C	3.175600	-4.518302	-1.868727
H	4.337803	-6.827700	2.715131
H	0.572653	-6.062522	-2.967544
H	3.875015	-5.085656	-2.493071
H	-1.530075	-5.124873	-1.241101
H	-0.621900	-6.380862	1.393814
H	-1.898239	-3.579418	-0.462924
H	3.768872	-3.907071	-1.180030
Si	0.381852	-4.405698	0.203911
H	0.537503	-5.556392	2.446161
H	2.622277	-3.837832	-2.526109
H	5.651416	-7.950905	0.193644
H	1.806362	-7.324504	-2.845485
Si	1.176791	-2.333033	1.005287
H	5.504402	-6.340948	-0.523248
C	1.101474	-6.718595	-2.266962
Si	1.995895	-5.689405	-0.943711
H	-0.565387	0.960246	3.022181
H	-0.375490	2.688469	3.348857
C	-0.224811	1.908552	2.593923
H	-1.393964	0.356621	-3.021374
H	-3.403956	-0.196985	-0.239569
H	-3.139645	3.336612	2.215531
C	-2.420328	-0.671257	-0.147807
Si	1.034759	-0.567268	-0.554121
H	-0.587043	1.886296	-2.657719
H	-3.642894	2.727038	0.632319

C	-1.365053	1.195355	-2.316684
H	-2.399969	-1.526276	-0.833287
Si	-1.034759	0.567268	-0.554121
H	-2.325102	1.717697	-2.381071
C	-3.004752	2.519103	1.498008
H	0.852397	1.825208	2.415933
H	-3.375165	1.601373	1.968585
H	-2.335276	-1.060332	0.872617
H	0.565387	-0.960246	3.022181
H	0.375490	-2.688469	3.348857
C	0.224811	-1.908552	2.593923
H	1.393964	-0.356621	-3.021374
H	3.403956	0.196985	-0.239569
H	3.139645	-3.336612	2.215531
C	2.420328	0.671257	-0.147807
H	0.587043	-1.886296	-2.657719
H	3.642894	-2.727038	0.632319
C	1.365053	-1.195355	-2.316684
H	2.399969	1.526276	-0.833287
H	2.325102	-1.717697	-2.381071
C	3.004752	-2.519103	1.498008
H	-0.852397	-1.825208	2.415933
H	3.375165	-1.601373	1.968585
H	2.335276	1.060332	0.872617

MP2/6311G optimized geometry, all-*gauche*-$Si_{16}Me_{34}$**

152
RI-MP2
Energy= -5977.51510354992934
TD B3LYP
Energy= -5990.19054257

Si	-1.137487	11.103008	-0.052604
Si	0.372451	9.770344	-1.272536
Si	1.604694	8.231656	0.014793
Si	0.453467	6.759181	1.448605
Si	-1.155274	5.299511	0.537211
Si	-0.500062	3.776249	-1.136016
Si	1.207348	2.223408	-0.664035
Si	0.927113	0.726395	1.133113
Si	-0.927113	-0.726395	1.133113
Si	-1.207348	-2.223408	-0.664035
Si	0.500062	-3.776249	-1.136016
Si	1.155274	-5.299511	0.537211
Si	-0.453467	-6.759181	1.448605
Si	-1.604694	-8.231656	0.014793
Si	-0.372451	-9.770344	-1.272536
Si	1.137487	-11.103008	-0.052604
C	-2.760989	10.166071	0.181325
C	-1.459257	12.647762	-1.095488
C	-0.366141	11.600319	1.598924
C	1.663620	10.965549	-1.997919
C	-0.525502	8.914734	-2.710791
C	2.735155	7.269574	-1.174034
C	2.720905	9.261403	1.161076
C	1.787643	5.758932	2.363118
C	-0.453467	7.787611	2.767728
C	-1.885170	4.345021	2.012503
C	-2.584019	6.318196	-0.196145
C	-2.082658	2.864744	-1.666493
C	0.097759	4.758051	-2.652249
C	1.480260	1.254313	-2.277489
C	2.831848	3.148559	-0.309947
C	2.535451	-0.285702	1.209043
C	0.822563	1.690242	2.770287
C	-0.822563	-1.690242	2.770287
C	-2.535451	0.285702	1.209043
C	-2.831848	-3.148559	-0.309947
C	-1.480260	-1.254313	-2.277489
C	-0.097759	-4.758051	-2.652249

C	2.082658	-2.864744	-1.666493
C	2.584019	-6.318196	-0.196145
C	1.885170	-4.345021	2.012503
C	0.453467	-7.787611	2.767728
C	-1.787643	-5.758932	2.363118
C	-2.720905	-9.261403	1.161076
C	-2.735155	-7.269574	-1.174034
C	-1.663620	-10.965549	-1.997919
C	0.525502	-8.914734	-2.710791
C	0.366141	-11.600319	1.598924
C	1.459257	-12.647762	-1.095488
C	2.760989	-10.166071	0.181325
H	-1.860262	12.375279	-2.076201
H	-3.165440	9.846053	-0.783388
H	2.416504	10.411106	-2.566073
H	-0.881751	7.127827	3.528392
H	-0.899426	9.664929	-3.414231
H	-1.261173	8.371380	2.325292
H	2.166024	11.524471	-1.202995
H	3.395172	8.605167	1.719650
H	-0.536068	13.216382	-1.240471
H	0.596057	12.096341	1.441251
H	-2.724518	3.540962	-2.239715
H	-2.185375	13.294606	-0.594216
H	-2.644051	2.528380	-0.794910
H	2.126505	9.836205	1.875876
H	-1.027234	12.293702	2.127264
H	3.330727	9.955902	0.575864
H	-2.617215	9.285446	0.807581
H	-0.209282	10.727795	2.236572
H	2.165009	6.880442	-2.017599
H	-0.531623	5.636203	-2.819571
H	-2.245553	6.906496	-1.047314
H	0.528848	0.922866	-2.693005
H	1.338442	4.933113	2.919760
H	3.681826	2.478936	-0.474301
H	0.050750	4.126635	-3.544880
H	2.522841	5.366669	1.660847
H	2.312224	6.404455	3.074383
H	2.865042	3.484125	0.726524
H	3.509722	7.934717	-1.568112
H	-2.996334	6.988748	0.561859
H	-2.511190	5.012903	2.612373
H	2.123800	0.388502	-2.104692
H	0.159389	8.252420	-3.247948

H	-3.499674	10.811538	0.665760
H	-2.505731	3.514979	1.666974
H	-1.841725	2.006554	-2.298202
H	-1.090955	3.963916	2.653882
H	0.244255	8.468678	3.263353
H	1.181758	11.678123	-2.673931
H	2.941345	4.008980	-0.974441
H	-3.386179	5.654150	-0.532034
H	-1.373766	8.330476	-2.355825
H	1.131559	5.076750	-2.519225
H	3.226121	6.442298	-0.655507
H	1.965116	1.897950	-3.018124
H	-2.797974	0.665373	0.221741
H	-2.433946	1.121157	1.905447
H	-3.356943	-0.349427	1.555214
H	3.356943	0.349427	1.555214
H	2.797974	-0.665373	0.221741
H	2.433946	-1.121157	1.905447
H	1.522443	2.529046	2.771131
H	1.079431	1.029957	3.604532
H	-0.189316	2.059994	2.935248
H	-1.079431	-1.029957	3.604532
H	0.189316	-2.059994	2.935248
H	-1.522443	-2.529046	2.771131
H	1.860262	-12.375279	-2.076201
H	3.165440	-9.846053	-0.783388
H	-2.416504	-10.411106	-2.566073
H	0.881751	-7.127827	3.528392
H	0.899426	-9.664929	-3.414231
H	1.261173	-8.371380	2.325292
H	-2.166024	-11.524471	-1.202995
H	-3.395172	-8.605167	1.719650
H	0.536068	-13.216382	-1.240471
H	-0.596057	-12.096341	1.441251
H	2.724518	-3.540962	-2.239715
H	2.185375	-13.294606	-0.594216
H	2.644051	-2.528380	-0.794910
H	-2.126505	-9.836205	1.875876
H	1.027234	-12.293702	2.127264
H	-3.330727	-9.955902	0.575864
H	2.617215	-9.285446	0.807581
H	0.209282	-10.727795	2.236572
H	-2.165009	-6.880442	-2.017599
H	0.531623	-5.636203	-2.819571
H	2.245553	-6.906496	-1.047314

H	-0.528848	-0.922866	-2.693005
H	-1.338442	-4.933113	2.919760
H	-3.681826	-2.478936	-0.474301
H	-0.050750	-4.126635	-3.544880
H	-2.522841	-5.366669	1.660847
H	-2.312224	-6.404455	3.074383
H	-2.865042	-3.484125	0.726524
H	-3.509722	-7.934717	-1.568112
H	2.996334	-6.988748	0.561859
H	2.511190	-5.012903	2.612373
H	-2.123800	-0.388502	-2.104692
H	-0.159389	-8.252420	-3.247948
H	3.499674	-10.811538	0.665760
H	2.505731	-3.514979	1.666974
H	1.841725	-2.006554	-2.298202
H	1.090955	-3.963916	2.653882
H	-0.244255	-8.468678	3.263353
H	-1.181758	-11.678123	-2.673931
H	-2.941345	-4.008980	-0.974441
H	3.386179	-5.654150	-0.532034
H	1.373766	-8.330476	-2.355825
H	-1.131559	-5.076750	-2.519225
H	-3.226121	-6.442298	-0.655507
H	-1.965116	-1.897950	-3.018124

MP2/6311G optimized geometry, all-*cisoid*-$Si_{16}Me_{34}$**

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RI-MP2
Energy= -5977.5883975900
TD B3LYP
Energy= -5990.186422

Si	9.520936	-0.783060	-1.122150
Si	8.429817	-1.098205	0.971303
Si	7.049992	0.642105	1.866091
Si	5.687920	2.155407	0.600304
Si	4.435651	1.671958	-1.384648
Si	3.281869	-0.365267	-1.891963
Si	2.074857	-1.725411	-0.332029
Si	0.718579	-0.957684	1.487999
Si	-0.718579	0.957684	1.487999
Si	-2.074857	1.725411	-0.332029
Si	-3.281869	0.365267	-1.891963
Si	-4.435651	-1.671958	-1.384648
Si	-5.687920	-2.155407	0.600304
Si	-7.049992	-0.642105	1.866091
Si	-8.429817	1.098205	0.971303
Si	-9.520936	0.783060	-1.122150
C	8.450962	-1.369102	-2.571958
C	11.110360	-1.825397	-1.123916
C	10.009597	1.028192	-1.406542
C	7.421280	-2.715189	0.872885
C	5.930416	-0.209922	3.156508
C	8.221229	1.802015	2.838154
C	4.475624	2.878468	1.889659
C	6.811886	3.611626	0.074713
C	3.154690	3.085403	-1.499782
C	5.620092	1.930730	-2.863639
C	2.077275	0.122656	-3.292542
C	4.527479	-1.578900	-2.680073
C	0.975346	-2.836155	-1.433222
C	3.335435	-2.900320	0.495959
C	-0.353625	-2.473741	1.937397
C	1.870122	-0.678542	2.987499
C	-1.870122	0.678542	2.987499
C	0.353625	2.473741	1.937397
C	-3.335435	2.900320	0.495959
C	-0.975346	2.836155	-1.433222
C	-4.527479	1.578900	-2.680073
C	-2.077275	-0.122656	-3.292542

C	-5.620092	-1.930730	-2.863639
C	-3.154690	-3.085403	-1.499782
C	-6.811886	-3.611626	0.074713
C	-4.475624	-2.878468	1.889659
C	-8.221229	-1.802015	2.838154
C	-5.930416	0.209922	3.156508
C	-9.783166	1.371976	2.292559
C	-7.421280	2.715189	0.872885
C	-10.009597	-1.028192	-1.406542
C	-11.110360	1.825397	-1.123916
C	-8.450962	1.369102	-2.571958
C	9.783166	-1.371976	2.292559
H	8.995137	-1.248095	-3.514724
H	7.518973	-0.806395	-2.654170
H	8.190015	-2.426637	-2.474228
H	11.801268	-1.509593	-0.337256
H	11.630831	-1.725702	-2.082557
H	10.899935	-2.888481	-0.973377
H	10.663170	1.397090	-0.610440
H	9.133537	1.680782	-1.444703
H	10.547718	1.139422	-2.353794
H	8.066313	-3.554799	0.594768
H	6.618533	-2.656332	0.133998
H	6.965897	-2.955325	1.838146
H	6.523959	-0.820564	3.844299
H	5.190186	-0.863760	2.689331
H	5.390437	0.529648	3.754680
H	8.773752	1.240743	3.597590
H	7.664767	2.591170	3.352876
H	8.951323	2.284662	2.183107
H	5.021167	3.284418	2.747355
H	3.773170	2.132250	2.268012
H	3.891232	3.695603	1.457031
H	7.306973	4.046311	0.947714
H	6.228279	4.405865	-0.400934
H	7.589617	3.305664	-0.629057
H	3.632149	4.060818	-1.364444
H	2.365751	2.994860	-0.750221
H	2.677356	3.086860	-2.484085
H	6.448800	1.219136	-2.865562
H	6.047244	2.937443	-2.835865
H	5.089863	1.825474	-3.815117
H	2.605986	0.641172	-4.098387
H	1.277588	0.780506	-2.945444
H	1.611017	-0.767237	-3.724745

H	5.300392	-1.896772	-1.977396
H	5.026393	-1.119546	-3.538456
H	4.017698	-2.477268	-3.041526
H	1.567889	-3.320608	-2.215384
H	0.177840	-2.272948	-1.923157
H	0.506775	-3.627582	-0.840724
H	3.881156	-3.472953	-0.260005
H	2.830339	-3.618531	1.149300
H	4.071064	-2.364229	1.099726
H	0.263253	-3.369114	2.060910
H	-1.105476	-2.691670	1.176106
H	-0.877909	-2.304133	2.882215
H	2.461511	-1.576501	3.188945
H	1.289755	-0.459176	3.889092
H	2.565741	0.148991	2.832184
H	-1.289755	0.459176	3.889092
H	-2.565741	-0.148991	2.832184
H	-2.461511	1.576501	3.188945
H	0.877909	2.304133	2.882215
H	-0.263253	3.369114	2.060910
H	1.105476	2.691670	1.176106
H	-2.830339	3.618531	1.149300
H	-4.071064	2.364229	1.099726
H	-3.881156	3.472953	-0.260005
H	-0.177840	2.272948	-1.923157
H	-0.506775	3.627582	-0.840724
H	-1.567889	3.320608	-2.215384
H	-4.017698	2.477268	-3.041526
H	-5.300392	1.896772	-1.977396
H	-5.026393	1.119546	-3.538456
H	-1.277588	-0.780506	-2.945444
H	-1.611017	0.767237	-3.724745
H	-2.605986	-0.641172	-4.098387
H	-5.089863	-1.825474	-3.815117
H	-6.448800	-1.219136	-2.865562
H	-6.047244	-2.937443	-2.835865
H	-2.677356	-3.086860	-2.484085
H	-3.632149	-4.060818	-1.364444
H	-2.365751	-2.994860	-0.750221
H	-6.228279	-4.405865	-0.400934
H	-7.589617	-3.305664	-0.629057
H	-7.306973	-4.046311	0.947714
H	-3.891232	-3.695603	1.457031
H	-5.021167	-3.284418	2.747355
H	-3.773170	-2.132250	2.268012

H	-7.664767	-2.591170	3.352876
H	-8.951323	-2.284662	2.183107
H	-8.773752	-1.240743	3.597590
H	-5.390437	-0.529648	3.754680
H	-6.523959	0.820564	3.844299
H	-5.190186	0.863760	2.689331
H	-9.344715	1.552153	3.278902
H	-10.450400	0.510387	2.378892
H	-10.394983	2.243279	2.039932
H	-6.618533	2.656332	0.133998
H	-6.965897	2.955325	1.838146
H	-8.066313	3.554799	0.594768
H	-9.133537	-1.680782	-1.444703
H	-10.547718	-1.139422	-2.353794
H	-10.663170	-1.397090	-0.610440
H	-10.899935	2.888481	-0.973377
H	-11.801268	1.509593	-0.337256
H	-11.630831	1.725702	-2.082557
H	-8.190015	2.426637	-2.474228
H	-8.995137	1.248095	-3.514724
H	-7.518973	0.806395	-2.654170
H	10.394983	-2.243279	2.039932
H	9.344715	-1.552153	3.278902
H	10.450400	-0.510387	2.378892

PBE0/POB-TZVP optimized geometry, *all*-[180.0]-$(SiMe_2)_\infty$

Energy (a.u): -7.382418880949E+02
Unit cell length (Å): 3.89663067

Si	-8.567146499662E-01	-8.729650093813E-04	6.741882990016E-01
Si	1.091600684344E+00	8.729650093811E-04	-6.741882990016E-01
C	-9.121570066877E-01	1.535602003971E+00	1.759364638816E+00
C	1.036158327622E+00	-1.535602003971E+00	-1.759364638816E+00
C	-9.122390292425E-01	-1.540151558635E+00	1.755380074756E+00
C	1.036076305067E+00	1.540151558635E+00	-1.755380074756E+00
H	-1.884469500570E+00	1.639451394735E+00	2.241150571805E+00
H	6.384583373964E-02	-1.639451394735E+00	-2.241150571805E+00
H	-7.335498804674E-01	2.438684718632E+00	1.175337863178E+00
H	1.214765453843E+00	-2.438684718632E+00	-1.175337863178E+00
H	-1.594628647990E-01	1.491362129774E+00	2.547543057859E+00
H	1.788852469511E+00	-1.491362129774E+00	-2.547543057859E+00
H	-1.884546564145E+00	-1.645155307688E+00	2.236926486337E+00
H	6.376877016489E-02	1.645155307688E+00	-2.236926486337E+00
H	-1.595155854040E-01	-1.498027379262E+00	2.543645627559E+00
H	1.788799748906E+00	1.498027379262E+00	-2.543645627559E+00
H	-7.337400071876E-01	-2.441733430682E+00	1.169006169160E+00
H	1.214575327122E+00	2.441733430682E+00	-1.169006169160E+00

PBE0/POB-TZVP optimized geometry, *all*-[163.0]-$(SiMe_2)_\infty$

Energy (a.u): -4.798590180463E+03
Unit cell length (Å): 24.87911044

Si	3.827638108978E+00	3.213556635215E-01	6.121341752382E-01
Si	8.265641573551E-05	7.337300985091E-05	6.913593172789E-01
Si	-3.827472796146E+00	-3.212257263742E-01	6.122023715139E-01
Si	-7.655028248708E+00	-5.689358830355E-01	3.927972402735E-01
Si	-1.148258370127E+01	-6.863096853141E-01	8.340699500638E-02
Si	9.568971287820E+00	-6.464582096155E-01	-2.450907876535E-01
Si	5.741415835258E+00	-4.585109487600E-01	-5.174412245261E-01
Si	1.913860382697E+00	-1.655243551995E-01	-6.712521127026E-01
Si	-1.913695069865E+00	1.653818733524E-01	-6.712872313238E-01
Si	-5.741250522427E+00	4.584011077870E-01	-5.175385351368E-01
Si	-9.568805974989E+00	6.464061727598E-01	-2.452279975655E-01
Si	1.148274901410E+01	6.863273735921E-01	8.326131893038E-02
Si	7.655193561539E+00	5.690192442760E-01	3.926764706669E-01
C	3.914430828215E+00	2.184980871869E+00	8.560387279811E-01
C	8.687537565282E-02	1.536883445873E+00	1.773395891513E+00
C	-3.740680076909E+00	5.367045438819E-01	2.284489428037E+00
C	-7.568235529471E+00	-5.864269011221E-01	2.272233967679E+00
C	-1.139579098203E+01	-1.575215010289E+00	1.739437088714E+00
C	9.655764007057E+00	-2.203140343998E+00	8.081561352143E-01
C	5.828208554495E+00	-2.326352775616E+00	-3.082636495262E-01
C	2.000653101934E+00	-1.916625821931E+00	-1.354063947140E+00
C	-1.826902350628E+00	-1.067822990286E+00	-2.089664512703E+00
C	-5.654457803190E+00	2.560521977103E-02	-2.346548121594E+00
C	-9.482013255752E+00	1.113167582555E+00	-2.065865834798E+00
C	1.156954173334E+01	1.945716667299E+00	-1.311918581632E+00
C	7.741986280776E+00	2.332525511993E+00	-2.574265917464E-01
C	3.742014005679E+00	-5.361817323490E-01	2.284708121989E+00
C	-8.554144688314E-02	-1.536522151399E+00	1.773832498025E+00
C	-3.913096899445E+00	-2.184863862662E+00	8.565932257621E-01
C	-7.740652352007E+00	-2.332679593453E+00	-2.568812314552E-01
C	-1.156820780457E+01	-1.946106541221E+00	-1.311507294301E+00
C	9.483347184521E+00	-1.113703933521E+00	-2.065682841398E+00
C	5.655791731959E+00	-2.616517623935E-02	-2.346635343708E+00
C	1.828236279398E+00	1.067367707595E+00	-2.090001968796E+00
C	-1.999319173164E+00	1.916379512794E+00	-1.354574330087E+00
C	-5.826874625726E+00	2.326371866489E+00	-3.088300367455E-01
C	-9.654430078288E+00	2.203420461391E+00	8.076634962091E-01
C	1.139712491080E+01	1.575691982684E+00	1.739131055582E+00
C	7.569569458240E+00	5.869914598912E-01	2.272184648923E+00
H	4.766416195999E+00	2.462637398815E+00	1.478735663816E+00

H 9.388607434373E-01 1.493354395477E+00 2.453800067445E+00
H -2.888694709125E+00 1.819618970066E-01 2.866728447119E+00
H -6.716250161686E+00 -1.171115879189E+00 2.622923887381E+00
H -1.054380561425E+01 -2.255905120940E+00 1.778239074704E+00
H 1.050774937484E+01 -2.823893686086E+00 5.261811201154E-01
H 6.680193922280E+00 -2.744962239359E+00 -8.464185879212E-01
H 2.852638469718E+00 -2.037193023975E+00 -2.025113997915E+00
H -9.749169828436E-01 -8.627274376362E-01 -2.739880196256E+00
H -4.802472435405E+00 5.093786076724E-01 -2.826972860770E+00
H -8.630027887967E+00 1.764792152641E+00 -2.266440111598E+00
H 1.242152710112E+01 2.615913083491E+00 -1.186693246423E+00
H 8.593971648561E+00 2.867759852083E+00 1.649107403030E-01
H 3.012670405146E+00 2.558996137027E+00 1.343049856258E+00
H -8.148850474160E-01 1.641732159741E+00 2.378436390023E+00
H -4.642440499978E+00 3.483671296752E-01 2.868951810100E+00
H -8.469995952540E+00 -1.024804611520E+00 2.702224945100E+00
H -1.229755140510E+01 -2.163205966450E+00 1.916450910518E+00
H 8.754003583988E+00 -2.806042903924E+00 6.916410680746E-01
H 4.926448131427E+00 -2.806049228593E+00 -6.916154078868E-01
H 1.098892678865E+00 -2.163223491549E+00 -1.916431128771E+00
H -2.728662773697E+00 -1.024829322261E+00 -2.702215573552E+00
H -6.556218226259E+00 3.483408942246E-01 -2.868954995660E+00
H -1.038377367882E+01 1.641710409807E+00 -2.378451402918E+00
H 1.066778131027E+01 2.558983855257E+00 -1.343073257215E+00
H 6.840225857708E+00 2.890024938567E+00 -1.321407075988E-05
H 4.014599115997E+00 2.699734076567E+00 -1.001394577373E-01
H 1.870436634348E-01 2.437032932204E+00 1.165959897478E+00
H -3.640511789127E+00 1.616036912504E+00 2.164951891521E+00
H -7.468067241689E+00 4.248263115048E-01 2.667979497715E+00
H -1.129562269425E+01 -8.637068777479E-01 2.559805153621E+00
H 9.755932294839E+00 -1.954375230105E+00 1.865210297829E+00
H 5.928376842277E+00 -2.597319770019E+00 7.433182410250E-01
H 2.100821389716E+00 -2.645249651719E+00 -5.488590668419E-01
H -1.726734062846E+00 -2.087184716924E+00 -1.715299376964E+00
H -5.554289515408E+00 -1.050970916784E+00 -2.488785271422E+00
H -9.381844967970E+00 2.260076548184E-01 -2.692120453311E+00
H 1.166971002112E+01 1.451210596389E+00 -2.278723282915E+00
H 7.842154568558E+00 2.343958679311E+00 -1.343298069996E+00
H 4.644665872232E+00 -3.482546831549E-01 2.867925142780E+00
H 8.171104196702E-01 -1.641155477198E+00 2.377579577762E+00
H -3.010445032892E+00 -2.558087329483E+00 1.342559184419E+00
H -6.838000485453E+00 -2.888992202878E+00 -2.533848260891E-05
H -1.066555593802E+01 -2.558063778723E+00 -1.342604056643E+00
H 1.038599905107E+01 -1.641113770874E+00 -2.377608365560E+00
H 6.558443598513E+00 -3.482043756819E-01 -2.867931251213E+00

H 2.730888145951E+00 1.024474445661E+00 -2.701245649532E+00
H -1.096667306611E+00 2.162458517758E+00 -1.915737223083E+00
H -4.924222759172E+00 2.805049403888E+00 -6.913564859609E-01
H -8.751778211734E+00 2.805037276096E+00 6.914056903456E-01
H 1.229977677736E+01 2.162424912715E+00 1.915775155336E+00
H 8.472221324794E+00 1.024427061875E+00 2.701263619832E+00
H 3.641091232668E+00 -1.615485675939E+00 2.165510344572E+00
H -1.864642198942E-01 -2.436804362540E+00 1.166710555502E+00
H -4.014019672456E+00 -2.699880536359E+00 -9.936856144725E-02
H -7.841575125018E+00 -2.344446616385E+00 -1.342683538490E+00
H -1.166913057758E+01 -1.451928230243E+00 -2.278405897955E+00
H 9.382424411510E+00 -2.267905841836E-01 -2.692172923966E+00
H 5.554868958949E+00 1.050302051589E+00 -2.489195577298E+00
H 1.727313506387E+00 2.086783144855E+00 -1.715973521929E+00
H -2.100241946175E+00 2.645207368097E+00 -5.496426124091E-01
H -5.927797398737E+00 2.597646461513E+00 7.426047957023E-01
H -9.755352851299E+00 1.954996055630E+00 1.864730394476E+00
H 1.129620213779E+01 8.644796136584E-01 2.559668732313E+00
H 7.468646685229E+00 -4.240786896937E-01 2.668217810929E+00
H 2.891044711791E+00 -1.808101128237E-01 2.868048429952E+00
H -9.365107407704E-01 -1.492947967841E+00 2.455504114997E+00
H -4.764066193332E+00 -2.463069435400E+00 1.480433399329E+00
H -8.591621645894E+00 -2.868931378513E+00 1.662132330311E-01
H -1.241917709846E+01 -2.617555717179E+00 -1.186084381868E+00
H 8.632377890634E+00 -1.766529586007E+00 -2.266664358747E+00
H 4.804822438072E+00 -5.108128156688E-01 -2.827978847304E+00
H 9.772669855105E-01 8.619250147769E-01 -2.741437462783E+00
H -2.850288467051E+00 2.037206211660E+00 -2.026865793442E+00
H -6.677843919613E+00 2.745788016447E+00 -8.479635972037E-01
H -1.050539937217E+01 2.825342877000E+00 5.251968400846E-01
H 1.054615561691E+01 2.257645733504E+00 1.778041010618E+00
H 6.718600164353E+00 1.172749160044E+00 2.623557413335E+00

PBE0/POB-TZVP optimized geometry, *all*-[148.8]-$(SiMe_2)_\infty$

Energy (a.u): -2.583845448692E+03
Unit cell length (Å): 13.53766152

Si	-9.174648994449E-01	-6.409783542963E-04	6.986325397021E-01
Si	-4.785368189690E+00	-5.466125576828E-01	4.350891266939E-01
Si	4.884390035923E+00	-6.809737322120E-01	-1.560852729155E-01
Si	1.016486745678E+00	-3.025477970529E-01	-6.297242784602E-01
Si	-2.851416544568E+00	3.037028001374E-01	-6.291680582901E-01
Si	-6.719319834813E+00	6.812589944161E-01	-1.548354575381E-01
Si	2.950438390801E+00	5.458132707486E-01	4.360914008079E-01
C	-8.551952247133E-01	1.523962145798E+00	1.800535804666E+00
C	-4.723098514959E+00	-4.575407210750E-01	2.314097295765E+00
C	4.946659710655E+00	-2.094506092848E+00	1.085096324171E+00
C	1.078756420409E+00	-2.154265656569E+00	-9.610043114552E-01
C	-2.789146869836E+00	-5.918192418820E-01	-2.283449099640E+00
C	-6.657050160081E+00	1.416279132854E+00	-1.886410141923E+00
C	3.012708065532E+00	2.357890433722E+00	-6.886587158354E-02
C	-9.797018635770E-01	-1.527255463137E+00	1.797750419063E+00
C	-4.847605153822E+00	-2.357766081342E+00	-7.317735027865E-02
C	4.822153071791E+00	-1.412830750634E+00	-1.889001082314E+00
C	9.542497815457E-01	5.959949517970E-01	-2.282368470768E+00
C	-2.913653508700E+00	2.156024299443E+00	-9.570658489007E-01
C	-6.781556798945E+00	2.092523374728E+00	1.088926877774E+00
C	2.888201426668E+00	4.533096691446E-01	2.314935455425E+00
H	-1.789297677308E+00	1.621871424838E+00	2.357121547182E+00
H	-5.657200967554E+00	-8.316515402781E-01	2.737671386863E+00
H	4.012557258060E+00	-2.658923932965E+00	1.056698833917E+00
H	1.446539678145E-01	-2.483972371965E+00	-1.419989493696E+00
H	-3.723249322431E+00	-4.385389510736E-01	-2.827396770050E+00
H	5.946508903183E+00	1.937123244541E+00	-2.105716610172E+00
H	2.078605612937E+00	2.854092126903E+00	2.016111059559E-01
H	-7.136244740989E-01	2.436164764703E+00	1.221346440904E+00
H	-4.581527764344E+00	5.640367879414E-01	2.666167359964E+00
H	5.088230461269E+00	-1.732822394394E+00	2.103309877069E+00
H	1.220327171024E+00	-2.724830970616E+00	-4.338284296163E-02
H	-2.647576119222E+00	-1.664986249541E+00	-2.157407397393E+00
H	-6.515479409467E+00	6.486270769676E-01	-2.646860178497E+00
H	3.154278816147E+00	2.473810984939E+00	-1.143173259085E+00
H	-4.651241597453E-02	1.455573368510E+00	2.528288640811E+00
H	-3.914415706220E+00	-1.069160505029E+00	2.714375268244E+00
H	5.755342519394E+00	-2.788794711381E+00	8.564819555242E-01
H	1.887439229148E+00	-2.408409619018E+00	-1.646359738753E+00
H	-1.980464061097E+00	-2.144429609316E-01	-2.909458970131E+00

H -5.848367351343E+00 2.141003620576E+00 -1.981676254853E+00
H 3.821390874271E+00 2.884230807275E+00 4.383490991579E-01
H -1.788335234597E+00 -1.460183811368E+00 2.525680229310E+00
H -5.656238524843E+00 -2.885066033149E+00 4.331181918136E-01
H 4.013519700771E+00 -2.137434687347E+00 -1.985590678119E+00
H 1.456164105255E-01 2.197285737491E-01 -2.909109268760E+00
H -3.722286879720E+00 2.411431737166E+00 -1.642009245010E+00
H 5.947471345894E+00 2.787277618253E+00 8.615572311173E-01
H 2.079568055648E+00 1.064246602695E+00 2.716353539648E+00
H -4.556626554845E-02 -1.626200049837E+00 2.354097133219E+00
H -3.913469555794E+00 -2.854426398394E+00 1.963411593930E-01
H 5.756288669820E+00 -1.933211449273E+00 -2.109263712086E+00
H 1.888385379574E+00 4.437511514778E-01 -2.826549987225E+00
H -1.979517910671E+00 2.486560084292E+00 -1.415386470872E+00
H -5.847421200917E+00 2.656938557052E+00 1.061591926670E+00
H 3.822337024697E+00 8.265881046826E-01 2.739169950901E+00
H -1.121325030809E+00 -2.438395496769E+00 1.216903276843E+00
H -4.989228321055E+00 -2.471728018088E+00 -1.147687583122E+00
H 4.680529904559E+00 -6.437989277237E-01 -2.648046284436E+00
H 8.126266143133E-01 1.668923886321E+00 -2.154372123269E+00
H -3.055276675932E+00 2.724912974123E+00 -3.841181209838E-02
H -6.923179966178E+00 1.728987014315E+00 2.106473377041E+00
H 2.746578259436E+00 -5.689014321794E-01 2.665141149042E+00

PBE0/POB-TZVP optimized geometry, *all*-[130.2]-$(SiMe_2)_\infty$

Energy (a.u): -4.798547917960E+03
Unit cell length (Å): 25.37636734

Si	-9.218667470081E-01	-6.766868841571E-04	7.368748022630E-01
Si	-1.068200803141E+01	-3.430419719859E-01	6.521557617405E-01
Si	4.934218023630E+00	-6.068204754095E-01	4.180356955322E-01
Si	-4.825923260767E+00	-7.315837208963E-01	8.814868935369E-02
Si	1.079030279427E+01	-6.887499524654E-01	-2.619321192489E-01
Si	1.030161509871E+00	-4.881318702614E-01	-5.520074359557E-01
Si	-8.729979774526E+00	-1.756886592072E-01	-7.156245014959E-01
Si	6.886246280510E+00	1.770027063935E-01	-7.153006179535E-01
Si	-2.873895003888E+00	4.891448850733E-01	-5.511099831449E-01
Si	-1.263403628829E+01	6.892298654177E-01	-2.606666927931E-01
Si	2.982189766751E+00	7.314205897152E-01	8.949219550347E-02
Si	-6.777951517647E+00	6.060516714826E-01	4.191495003080E-01
Si	8.838274537389E+00	3.418436190277E-01	6.527847058911E-01
C	-7.352492408240E-01	1.490558636355E+00	1.870495371796E+00
C	-1.049539052522E+01	4.505615836762E-01	2.348938535517E+00
C	5.120835529815E+00	-6.926536979675E-01	2.289268188530E+00
C	-4.639305754583E+00	-1.677190364789E+00	1.705154088223E+00
C	1.097692030045E+01	-2.277502931372E+00	7.304097356380E-01
C	1.216779016056E+00	-2.356067023263E+00	-4.116626849897E-01
C	-8.543362268342E+00	-1.894884553811E+00	-1.459428145559E+00
C	7.072863786694E+00	-9.996068689148E-01	-2.172856205997E+00
C	-2.687277497704E+00	1.246687030810E-01	-2.388509095397E+00
C	-1.244741878210E+01	1.220384177622E+00	-2.056983335696E+00
C	3.168807272935E+00	2.036524344293E+00	-1.254227483124E+00
C	-6.591334011463E+00	2.386121326466E+00	-1.641432292480E-01
C	9.024892043574E+00	2.189086668624E+00	9.635442603086E-01
C	-1.108458287391E+00	-1.493983510246E+00	1.867770970238E+00
C	-1.086859957179E+01	-2.190853151314E+00	9.595403042752E-01
C	4.747626483248E+00	-2.385824738059E+00	-1.685094816832E-01
C	-5.012514801150E+00	-2.034232629620E+00	-1.257955776147E+00
C	1.060371125389E+01	-1.216622340895E+00	-2.059219562307E+00
C	8.435699694889E-01	-1.202985357601E-01	-2.388740963028E+00
C	-8.916571314909E+00	1.003584214163E+00	-2.171030596568E+00
C	6.699654740128E+00	1.897557915122E+00	-1.455963284190E+00
C	-3.060486544270E+00	2.356823965779E+00	-4.073523296633E-01
C	1.255573951077E+01	2.276170048683E+00	7.345781344613E-01
C	2.795598226368E+00	1.674073004257E+00	1.708225600607E+00
C	-6.964543058029E+00	6.884660093224E-01	2.290539168004E+00
C	8.651682997007E+00	-4.548602514333E-01	2.348117816000E+00
H	-1.646066854368E+00	1.624660982300E+00	2.457427147958E+00

H -1.140620813877E+01 2.965425171555E-01 2.930961280953E+00
H 4.210017916270E+00 -1.099510264944E+00 2.733047506394E+00
H -5.550123368127E+00 -2.243678495880E+00 1.909025484914E+00
H 1.006610268691E+01 -2.873847022667E+00 6.476687310905E-01
H 3.059614025114E-01 -2.845651830172E+00 -7.620611237712E-01
H -9.454179881886E+00 -2.165552097207E+00 -1.997211959009E+00
H 6.162046173150E+00 -9.893504765033E-01 -2.774825603451E+00
H -3.598095111248E+00 4.134994154013E-01 -2.916760142416E+00
H 1.201813094379E+01 1.721621574446E+00 -2.390500083524E+00
H 2.257989659391E+00 2.635340978574E+00 -1.316605264145E+00
H -7.502151625007E+00 2.945335523812E+00 5.890795443535E-02
H 8.114074430029E+00 2.580589195686E+00 1.420926070573E+00
H -5.565892373154E-01 2.413394884512E+00 1.319491821051E+00
H -1.031673052171E+01 1.523756618207E+00 2.289912509874E+00
H 5.299495533323E+00 2.850440739293E-01 2.735741839123E+00
H -4.460645751074E+00 -1.018968632533E+00 2.554845682292E+00
H 1.115558030396E+01 -2.089547905184E+00 1.788665168875E+00
H 1.395439019564E+00 -2.681436934541E+00 6.127230210221E-01
H -8.364702264834E+00 -2.659041077012E+00 -7.035865868346E-01
H 7.251523790203E+00 -2.027490953658E+00 -1.858712986785E+00
H -2.508617494195E+00 -9.314670867363E-01 -2.588030641383E+00
H -1.226875877859E+01 3.779446643615E-01 -2.724461665190E+00
H 3.347467276444E+00 1.600773847581E+00 -2.236751354825E+00
H -6.412674007954E+00 2.456885033736E+00 -1.236628264845E+00
H 9.203552047082E+00 2.750153467336E+00 4.679145762479E-02
H 8.846014293370E-02 1.345572630505E+00 2.568996308147E+00
H -9.671681141464E+00 -2.426719655663E-03 2.900052041993E+00
H 5.944544913572E+00 -1.349870137589E+00 2.566740802435E+00
H -3.815596370825E+00 -2.388074574699E+00 1.645420177618E+00
H 1.180062968421E+01 -2.879199906164E+00 3.471536195724E-01
H 2.040488399813E+00 -2.710735237247E+00 -1.030641649063E+00
H -7.719652884584E+00 -1.921273793378E+00 -2.172329336476E+00
H 7.896573170452E+00 -6.916716773053E-01 -2.816362552310E+00
H -1.863568113946E+00 6.963840844910E-01 -2.815201048257E+00
H -1.162370939834E+01 1.924906644868E+00 -2.169110910899E+00
H 3.992516656693E+00 2.712456290546E+00 -1.026103604474E+00
H -5.767624627705E+00 2.878614888702E+00 3.519716718467E-01
H 9.848601427331E+00 2.385317506926E+00 1.649414479866E+00
H -1.932155360889E+00 -1.350281622199E+00 2.566552473652E+00
H -1.169229664529E+01 -2.388351405477E+00 1.645062194329E+00
H 3.923929409749E+00 -2.879278664515E+00 3.467079914349E-01
H -5.836211874648E+00 -2.710597880582E+00 -1.031072834013E+00
H 9.780014180388E+00 -1.920951788453E+00 -2.172647298963E+00
H 1.987289599006E-02 -6.912387915687E-01 -2.816494450960E+00
H -9.740268388408E+00 6.968286821338E-01 -2.815116666679E+00

H 5.875957666629E+00 1.925261102456E+00 -2.168829579895E+00
H -3.884183617769E+00 2.712639406116E+00 -1.025689773587E+00
H 1.173204243727E+01 2.878584712684E+00 3.524231989475E-01
H 1.971901152870E+00 2.385080952283E+00 1.649800263763E+00
H -7.788240131528E+00 1.345183889055E+00 2.569227970399E+00
H 7.827985923508E+00 -2.878591932488E-03 2.900076511571E+00
H -1.976273736438E-01 -1.629148345714E+00 2.454439111252E+00
H -9.957768658041E+00 -2.583173948765E+00 1.416194913707E+00
H 5.658457396995E+00 -2.945425530774E+00 5.351752843063E-02
H -4.101683887403E+00 -2.632915619909E+00 -1.321420077653E+00
H 1.151454216763E+01 -1.717236470596E+00 -2.393636268785E+00
H 1.754400883236E+00 -4.081591408117E-01 -2.917499237182E+00
H -8.005740401162E+00 9.944225292814E-01 -2.772998290018E+00
H 7.610485653874E+00 2.169193982007E+00 -1.993236852863E+00
H -2.149655630523E+00 2.847029235076E+00 -7.568488738254E-01
H -1.190979691492E+01 2.872644400810E+00 6.529240611882E-01
H 3.706429140115E+00 2.240171353438E+00 1.913119962371E+00
H -6.053712144282E+00 1.094502045983E+00 2.735043135770E+00
H 9.562513910754E+00 -3.019044900259E-01 2.930400887607E+00
H -1.287117853108E+00 -2.415815225230E+00 1.315089322414E+00
H -1.104725913751E+01 -2.750250629477E+00 4.176845026284E-02
H 4.568966917530E+00 -2.454636758625E+00 -1.241121070479E+00
H -5.191174366867E+00 -1.596695187951E+00 -2.239684711104E+00
H 1.042505168817E+01 -3.729699919806E-01 -2.725163575542E+00
H 6.649104037714E-01 9.361981343770E-01 -2.586340306605E+00
H -9.095230880626E+00 2.030894550559E+00 -1.855017642204E+00
H 6.520995174410E+00 2.660337500141E+00 -6.987327913599E-01
H -3.239146109988E+00 2.680329188983E+00 6.176233213414E-01
H 1.237707994505E+01 2.086289762097E+00 1.792489374291E+00
H 2.616938660651E+00 1.014306493232E+00 2.556717713430E+00
H -7.143202623747E+00 -2.900421695141E-01 2.735232836210E+00
H 8.473023431289E+00 -1.527945666612E+00 2.287139079344E+00

PBE0/POB-TZVP optimized geometry, *all*-[111.6]-$(SiMe_2)_\infty$

Energy (a.u): -1.291915390623E+04
Unit cell length (Å): 66.32182610

Si	-4.984376484195E-01	-7.599448046794E-04	8.289679964959E-01
Si	-6.183165599671E+00	-1.487656835208E-01	8.155104463691E-01
Si	-1.186789355092E+01	-2.919899707637E-01	7.758417194918E-01
Si	-1.755262150217E+01	-4.258294600962E-01	7.112368013853E-01
Si	-2.323734945342E+01	-5.459824402075E-01	6.237721472747E-01
Si	-2.892207740468E+01	-6.485870954547E-01	5.162589431092E-01
Si	3.171502074200E+01	-7.303456277947E-01	3.921527517330E-01
Si	2.603029279075E+01	-7.886302507270E-01	2.554424482517E-01
Si	2.034556483950E+01	-8.215676485139E-01	1.105220143048E-01
Si	1.466083688825E+01	-8.280991860893E-01	-3.795068811963E-02
Si	8.976108936999E+00	-8.080149344616E-01	-1.852036242020E-01
Si	3.291380985748E+00	-7.619604180034E-01	-3.265039634164E-01
Si	-2.393346965503E+00	-6.914158667675E-01	-4.573101965983E-01
Si	-8.078074916754E+00	-5.986486406747E-01	-5.734181037854E-01
Si	-1.376280286801E+01	-4.866403547010E-01	-6.710958813069E-01
Si	-1.944753081926E+01	-3.589910473181E-01	-7.472040850237E-01
Si	-2.513225877051E+01	-2.198034722956E-01	-7.992965346462E-01
Si	-3.081698672176E+01	-7.355123281864E-02	-8.256989359818E-01
Si	2.982011142492E+01	7.506500379928E-02	-8.255626941276E-01
Si	2.413538347367E+01	2.212685894314E-01	-7.988921880089E-01
Si	1.845065552242E+01	3.603604205388E-01	-7.465446296369E-01
Si	1.276592757117E+01	4.878699712245E-01	-6.702025126094E-01
Si	7.081199619916E+00	5.996989796144E-01	-5.723195353822E-01
Si	1.396471668664E+00	6.922531693654E-01	-4.560417373817E-01
Si	-4.288256282587E+00	7.625577726653E-01	-3.251063827094E-01
Si	-9.972984233838E+00	8.083531417170E-01	-1.837218413984E-01
Si	-1.565771218509E+01	8.281673756788E-01	-3.643232893797E-02
Si	-2.134244013634E+01	8.213636287679E-01	1.120281485511E-01
Si	-2.702716808759E+01	7.881605790082E-01	2.568879491687E-01
Si	-3.271189603884E+01	7.296253997384E-01	3.934911597319E-01
Si	2.792520210784E+01	6.476394597833E-01	5.174472406557E-01
Si	2.224047415659E+01	5.448378547112E-01	6.247721415078E-01
Si	1.655574620533E+01	4.245247126946E-01	7.120163516677E-01
Si	1.087101825408E+01	2.905669971119E-01	7.763757704359E-01
Si	5.186290302832E+00	1.472702191627E-01	8.157818331382E-01
C	-8.824958371825E-01	1.441831902150E+00	1.976080161649E+00
C	-6.567223788434E+00	1.065818332773E+00	2.201772767758E+00
C	-1.225195173968E+01	6.555484852233E-01	2.356698585488E+00
C	-1.793667969094E+01	2.242087699712E-01	2.435878171581E+00
C	-2.362140764219E+01	-2.143371996273E-01	2.436766628993E+00

C -2.930613559344E+01 -6.459941952726E-01 2.359335401971E+00
C 3.133096255324E+01 -1.056888405956E+00 2.206073193861E+00
C 2.564623460199E+01 -1.433813353661E+00 1.981905978138E+00
C 1.996150665074E+01 -1.764654360434E+00 1.694038673560E+00
C 1.427677869949E+01 -2.038777924101E+00 1.351723572154E+00
C 8.592050748236E+00 -2.247373487774E+00 9.659629629372E-01
C 2.907322796985E+00 -2.383736618406E+00 5.491555092946E-01
C -2.777405154266E+00 -2.443484492777E+00 1.146977457365E-01
C -8.462133105517E+00 -2.424696765044E+00 -3.234464977431E-01
C -1.414686105677E+01 -2.327977288236E+00 -7.511949046526E-01
C -1.983158900802E+01 -2.156434705917E+00 -1.154799289241E+00
C -2.551631695927E+01 -1.915582537831E+00 -1.521287474502E+00
C -3.120104491052E+01 -1.613161970831E+00 -1.838880228612E+00
C 2.943605323616E+01 -1.258893050775E+00 -2.097369859140E+00
C 2.375132528491E+01 -8.641622722467E-01 -2.288448296672E+00
C 1.806659733365E+01 -4.416566072531E-01 -2.405974123009E+00
C 1.238186938240E+01 -4.955735506159E-03 -2.446169961389E+00
C 6.697141431152E+00 4.319044176576E-01 -2.407743884495E+00
C 1.012413479901E+00 8.548828074657E-01 -2.291930938056E+00
C -4.672314471350E+00 1.250384560442E+00 -2.102453445460E+00
C -1.035704242260E+01 1.605697924826E+00 -1.845401369222E+00
C -1.604177037385E+01 1.909402836733E+00 -1.529036574577E+00
C -2.172649832510E+01 2.151737970406E+00 -1.163527286329E+00
C -2.741122627635E+01 2.324914475254E+00 -7.606212737450E-01
C -3.309595422761E+01 2.423366315921E+00 -3.332682675815E-01
C 2.754114391907E+01 2.443929169242E+00 1.047962549160E-01
C 2.185641596782E+01 2.385942128192E+00 5.394925395539E-01
C 1.617168801657E+01 2.251268943983E+00 9.568490900746E-01
C 1.048696006532E+01 2.044238123563E+00 1.343451723542E+00
C 4.802232114069E+00 1.771503807848E+00 1.686874713219E+00
C -1.143890209342E-01 -1.445446294502E+00 1.973444816666E+00
C -5.799116972185E+00 -1.774589556411E+00 1.683636344640E+00
C -1.148384492344E+01 -2.046696049840E+00 1.339714415196E+00
C -1.716857287469E+01 -2.253020048200E+00 9.527329621278E-01
C -2.285330082594E+01 -2.386930128419E+00 5.351298877451E-01
C -2.853802877719E+01 -2.444122310339E+00 1.003272984640E-01
C 3.209906936949E+01 -2.422758390174E+00 -3.376998927393E-01
C 2.641434141824E+01 -2.323525021896E+00 -7.648731315296E-01
C 2.072961346699E+01 -2.149611647612E+00 -1.167462718533E+00
C 1.504488551574E+01 -1.906607986268E+00 -1.532529093171E+00
C 9.360157564484E+00 -1.602324375482E+00 -1.848338721785E+00
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C -2.009298338018E+00 -8.506922611922E-01 -2.293495609645E+00
C -7.694026289269E+00 -4.275018322863E-01 -2.408535160239E+00
C -1.337875424052E+01 9.428857258897E-03 -2.446162409033E+00

C -1.906348219177E+01 4.460564955738E-01 -2.405167985291E+00
C -2.474821014302E+01 8.683475111044E-01 -2.286869483524E+00
C -3.043293809427E+01 1.262729123149E+00 -2.095069114914E+00
C 3.020416005241E+01 1.616525582199E+00 -1.835931501121E+00
C 2.451943210115E+01 1.918365578956E+00 -1.517785538273E+00
C 1.883470414990E+01 2.158547727568E+00 -1.150856699387E+00
C 1.314997619865E+01 2.329352376157E+00 -7.469383792550E-01
C 7.465248247401E+00 2.425289722780E+00 -3.190128450304E-01
C 1.780520296150E+00 2.443276262176E+00 1.191660245181E-01
C -3.904207655102E+00 2.382733892173E+00 5.535147999885E-01
C -9.588935606353E+00 2.245608494354E+00 9.700731543537E-01
C -1.527366355760E+01 2.036307391835E+00 1.355452559359E+00
C -2.095839150886E+01 1.761557694262E+00 1.697266603837E+00
C -2.664311946011E+01 1.430190082982E+00 1.984529103151E+00
C -3.232784741136E+01 1.052854985670E+00 2.208007204215E+00
C 2.830925073532E+01 6.416802628265E-01 2.360518136980E+00
C 2.262452278407E+01 2.098814083596E-01 2.437160074583E+00
C 1.693979483282E+01 -2.286632072629E-01 2.435469682086E+00
C 1.125506688157E+01 -6.598583992592E-01 2.355501290095E+00
C 5.570338930317E+00 -1.069845199370E+00 2.199825148529E+00
H -1.724659479090E+00 1.199868672547E+00 2.626539653852E+00
H -7.409387430341E+00 7.115995246943E-01 2.798574905389E+00
H -1.309411538159E+01 2.004589826117E-01 2.880661656791E+00
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H -3.014829923535E+01 -1.305405510430E+00 2.575715791379E+00
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H 2.480407096008E+01 -2.127207842269E+00 1.952788309164E+00
H 1.911934300883E+01 -2.441706553791E+00 1.541578570749E+00
H 1.343461505758E+01 -2.677726807631E+00 1.080821228656E+00
H 7.749887106329E+00 -2.827682718633E+00 5.853254029702E-01
H 2.065159155077E+00 -2.886754580433E+00 7.101673722588E-02
H -3.619568796174E+00 -2.853043774789E+00 -4.455744648856E-01
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H -5.514478113258E+00 1.943597734416E+00 -2.135608398417E+00

H -1.119920606451E+01 2.293690923353E+00 -1.754245516667E+00
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H -2.825338991826E+01 2.868767463939E+00 -3.294975302842E-01
H 3.238370822842E+01 2.881499246430E+00 1.880358408435E-01
H 2.669898027717E+01 2.801617272235E+00 6.995255853301E-01
H 2.101425232591E+01 2.631689013733E+00 1.188532001933E+00
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H -1.817478439497E+01 1.285783641849E+00 2.447171487390E+00
H -2.385951234623E+01 8.281612279231E-01 2.637429969289E+00
H -2.954424029748E+01 3.439210307186E-01 2.742919281891E+00
H 3.109285784920E+01 -1.513730713924E-01 2.760248911891E+00
H 2.540812989795E+01 -6.418019184386E-01 2.688861870723E+00
H 1.972340194670E+01 -1.111602723750E+00 2.531052596627E+00
H 1.403867399545E+01 -1.545675702890E+00 2.291893209518E+00
H 8.353946044198E+00 -1.930069393153E+00 1.979070488879E+00
H 2.669218092947E+00 -2.252429065054E+00 1.602638814343E+00
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H -1.438496576081E+01 -2.755587303389E+00 2.205141168784E-01
H -2.006969371206E+01 -2.750678197740E+00 -2.750587479392E-01
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H 1.214376467837E+01 -1.061244694023E+00 -2.552576651493E+00
H 6.459036727114E+00 -5.884098945667E-01 -2.701048251756E+00
H 7.743087758629E-01 -9.666311695349E-02 -2.762705938778E+00
H -4.910419175388E+00 3.981904927733E-01 -2.735567983766E+00
H -1.059514712664E+01 8.802459324300E-01 -2.620506622922E+00
H -1.627987507789E+01 1.334009543550E+00 -2.421220023058E+00
H -2.196460302914E+01 1.744896990313E+00 -2.144113419466E+00
H -2.764933098039E+01 2.099702012102E+00 -1.798093246390E+00
H -3.333405893164E+01 2.387020883581E+00 -1.394280876900E+00
H 2.730303921504E+01 2.597618939814E+00 -9.456551728070E-01
H 2.161831126378E+01 2.724727385994E+00 -4.666353333728E-01
H 1.593358331253E+01 2.764260852075E+00 2.738254962483E-02
H 1.024885536128E+01 2.714948699929E+00 5.205203349471E-01
H 4.564127410031E+00 2.578375862700E+00 9.969281684186E-01

H -2.116333993329E-02 1.640212136469E+00 2.616581984801E+00
H -5.705891291184E+00 1.146644498458E+00 2.867403621739E+00
H -1.139061924244E+01 6.162227628048E-01 3.026064546967E+00
H -1.707534719369E+01 6.599512052508E-02 3.087465267800E+00
H -2.276007514494E+01 -4.863536592293E-01 3.049632314552E+00
H -2.844480309619E+01 -1.023070632203E+00 2.913781669468E+00
H 3.219229505049E+01 -1.526905273272E+00 2.684279684061E+00
H 2.650756709924E+01 -1.981663922517E+00 2.368502740974E+00
H 2.082283914799E+01 -2.372730262773E+00 1.976600170982E+00
H 1.513811119674E+01 -2.687535100095E+00 1.521168045143E+00
H 9.453383245485E+00 -2.915960347988E+00 1.016844326712E+00
H 3.768655294234E+00 -3.050664231037E+00 4.798383949576E-01
H -1.916072657017E+00 -3.087317255606E+00 -7.258993762285E-02
H -7.600800608268E+00 -3.024741363326E+00 -6.226851698809E-01
H -1.328552855952E+01 -2.864947794864E+00 -1.152766788432E+00
H -1.897025651077E+01 -2.613072446987E+00 -1.645797533903E+00
H -2.465498446202E+01 -2.277210800622E+00 -2.085930992468E+00
H -3.033971241327E+01 -1.868157725429E+00 -2.459020912625E+00
H 3.029738573341E+01 -1.399060523815E+00 -2.753075877361E+00
H 2.461265778216E+01 -8.849963658156E-01 -2.958644718161E+00
H 1.892792983090E+01 -3.424876964411E-01 -3.069120283337E+00
H 1.324320187965E+01 2.110288092969E-01 -3.080951797327E+00
H 7.558473928402E+00 7.577626754689E-01 -2.993758985535E+00
H 1.873745977150E+00 1.280141425762E+00 -2.810344296675E+00
H -3.810981974101E+00 1.761375377328E+00 -2.536602829761E+00
H -9.495709925352E+00 2.185997275001E+00 -2.181332860774E+00
H -1.518043787660E+01 2.540359421612E+00 -1.755953058836E+00
H -2.086516582785E+01 2.813072326197E+00 -1.274135480783E+00
H -2.654989377911E+01 2.995370771615E+00 -7.513661400163E-01
H -3.223462173036E+01 3.081395535833E+00 -2.044472732831E-01
H 2.840247641632E+01 3.068381712150E+00 3.490426970332E-01
H 2.271774846507E+01 2.956747575565E+00 8.913141478736E-01
H 1.703302051382E+01 2.750081139081E+00 1.404938028626E+00
H 1.134829256257E+01 2.455024832013E+00 1.873406045151E+00
H 5.663564611318E+00 2.081062006843E+00 2.281661249941E+00
H -9.757246586567E-01 -1.644989178362E+00 2.613581319686E+00
H -6.660452609908E+00 -2.085226490261E+00 2.277855832982E+00
H -1.234518056116E+01 -2.458442907034E+00 1.868918185580E+00
H -1.802990851241E+01 -2.752642945961E+00 1.399911969942E+00
H -2.371463646366E+01 -2.958370775723E+00 8.859114317395E-01
H -2.939936441491E+01 -3.069014134597E+00 3.434369711901E-01
H 3.123773373177E+01 -3.081016853992E+00 -2.100758361941E-01
H 2.555300578052E+01 -2.993993156631E+00 -7.568366333521E-01
H 1.986827782926E+01 -2.810740055750E+00 -1.279272078387E+00
H 1.418354987801E+01 -2.537147456792E+00 -1.760590666234E+00

H 8.498821926762E+00 -2.182008851002E+00 -2.185322421449E+00
H 2.814093975511E+00 -1.756738685377E+00 -2.539816115950E+00
H -2.870633975740E+00 -1.275005492954E+00 -2.812678030716E+00
H -8.555361926992E+00 -7.522925749107E-01 -2.995138159296E+00
H -1.424008987824E+01 -2.054003545209E-01 -3.081332083028E+00
H -1.992481782949E+01 3.480936022672E-01 -3.068489458284E+00
H -2.560954578075E+01 8.903995442661E-01 -2.957023057588E+00
H -3.129427373200E+01 1.404087312289E+00 -2.750515502775E+00
H 2.934282441468E+01 1.872646558808E+00 -2.455604116571E+00
H 2.365809646343E+01 2.281017404108E+00 -2.081767593583E+00
H 1.797336851218E+01 2.616074473213E+00 -1.641021347253E+00
H 1.228864056093E+01 2.867048756236E+00 -1.147531324585E+00
H 6.603912609678E+00 3.025873733217E+00 -6.171587009531E-01
H 9.191846584270E-01 3.087444638716E+00 -6.695008887282E-02
H -4.765543292824E+00 3.049782533169E+00 4.854103541506E-01
H -1.045027124408E+01 2.914097907636E+00 1.022169308995E+00
H -1.613499919533E+01 2.684751777624E+00 1.526074901204E+00
H -2.181972714658E+01 2.369115516457E+00 1.980931190430E+00
H -2.750445509783E+01 1.977333933278E+00 2.372118721280E+00
H 3.313264304885E+01 1.521999210527E+00 2.687064404642E+00
H 2.744791509760E+01 1.017746180844E+00 2.915645627115E+00
H 2.176318714635E+01 4.807819515049E-01 3.050515600131E+00
H 1.607845919510E+01 -7.163500534434E-02 3.087339491787E+00
H 1.039373124385E+01 -6.217495541804E-01 3.024933751905E+00
H 4.709003292595E+00 -1.151880560768E+00 2.865304152313E+00
H 7.277744363076E-01 -1.204676837800E+00 2.624347983650E+00
H -4.956953514944E+00 -1.653912612242E+00 2.367070276499E+00
H -1.064168146619E+01 -2.049990274483E+00 2.033712983029E+00
H -1.632640941745E+01 -2.380179562565E+00 1.634990480940E+00
H -2.201113736870E+01 -2.633867921087E+00 1.183718039520E+00
H -2.769586531995E+01 -2.802901597472E+00 6.943999263421E-01
H 3.294123282673E+01 -2.881847710280E+00 1.827632281779E-01
H 2.725650487548E+01 -2.868168866486E+00 -3.347476305180E-01
H 2.157177692423E+01 -2.762304715387E+00 -8.414994249378E-01
H 1.588704897298E+01 -2.567657817903E+00 -1.321204735452E+00
H 1.020232102173E+01 -2.290484285475E+00 -1.758445438678E+00
H 4.517593070475E+00 -1.939692703496E+00 -2.139168258651E+00
H -1.167134880776E+00 -1.526557802042E+00 -2.451136450678E+00
H -6.851862832027E+00 -1.064358076775E+00 -2.684323100378E+00
H -1.253659078328E+01 -5.679490071628E-01 -2.831233396963E+00
H -1.822131873453E+01 -5.328558915075E-02 -2.887145522624E+00
H -2.390604668578E+01 4.630904715402E-01 -2.850262415636E+00
H -2.959077463703E+01 9.645824234436E-01 -2.721769529406E+00
H 3.104632350965E+01 1.435071902597E+00 -2.505796731021E+00
H 2.536159555840E+01 1.859436990019E+00 -2.209285563925E+00

H 1.967686760715E+01 2.224038242632E+00 -1.841766140998E+00
H 1.399213965589E+01 2.517157076183E+00 -1.415050838889E+00
H 8.307411704643E+00 2.729372410181E+00 -9.428546385107E-01
H 2.622683753391E+00 2.853863469181E+00 -4.403543142672E-01
H -3.062044197860E+00 2.886629008114E+00 7.629935996160E-02
H -8.746772149111E+00 2.826615915601E+00 5.905007099819E-01
H -1.443150010036E+01 2.675753061813E+00 1.085722881318E+00
H -2.011622805161E+01 2.438889303001E+00 1.546049025912E+00
H -2.580095600286E+01 2.123637635266E+00 1.956683882721E+00
H -3.148568395412E+01 1.740130506599E+00 2.304429309574E+00
H 2.915141419256E+01 1.300694151665E+00 2.578108482326E+00
H 2.346668624131E+01 8.194524164824E-01 2.768925127182E+00
H 1.778195829006E+01 3.118728063862E-01 2.870746240171E+00
H 1.209723033881E+01 -2.057306523171E-01 2.880299206943E+00
H 6.412502387559E+00 -7.167217585791E-01 2.797276987285E+00
H 1.237113824356E-01 -2.361571804345E+00 1.436989500774E+00
H -5.561016568816E+00 -2.580204757012E+00 9.922215600892E-01
H -1.124574452007E+01 -2.715907805789E+00 5.155628020606E-01
H -1.693047247132E+01 -2.764319343031E+00 2.233343136721E-02
H -2.261520042257E+01 -2.723883382099E+00 -4.716137541863E-01
H -2.829992837382E+01 -2.595899568047E+00 -9.504028856352E-01
H 3.233716977286E+01 -2.384481405966E+00 -1.398645286346E+00
H 2.665244182161E+01 -2.096424049538E+00 -1.801934076744E+00
H 2.096771387036E+01 -1.740985899215E+00 -2.147307223279E+00
H 1.528298591911E+01 -1.329591029603E+00 -2.423664148848E+00
H 9.598257967854E+00 -8.754620103090E-01 -2.622122514475E+00
H 3.913530016603E+00 -3.931949216708E-01 -2.736303704998E+00
H -1.771197934648E+00 1.017097752718E-01 -2.762537843004E+00
H -7.455925885899E+00 5.933454363501E-01 -2.699981741711E+00
H -1.314065383715E+01 1.065910486898E+00 -2.550646005688E+00
H -1.882538178840E+01 1.504216297363E+00 -2.319330408364E+00
H -2.451010973965E+01 1.894175358357E+00 -2.013469623363E+00
H -3.019483769090E+01 2.223254064801E+00 -1.642894267979E+00
H 3.044226045578E+01 2.480875556303E+00 -1.219514939045E+00
H 2.475753250452E+01 2.658759666154E+00 -7.569393965488E-01
H 1.907280455327E+01 2.751189052700E+00 -2.700351990362E-01
H 1.338807660202E+01 2.755192959406E+00 2.255481519593E-01
H 7.703348650771E+00 2.670642697417E+00 7.138821997691E-01
H 2.018620699519E+00 2.500255781720E+00 1.179271486294E+00
H -3.666107251732E+00 2.249508587982E+00 1.606758016942E+00
H -9.350835202983E+00 1.926460337325E+00 1.982602022880E+00
H -1.503556315423E+01 1.541494066328E+00 2.294723568513E+00
H -2.072029110549E+01 1.106982907695E+00 2.533090810548E+00
H -2.640501905674E+01 6.368924075795E-01 2.690042429699E+00
H -3.208974700799E+01 1.463316614477E-01 2.760533871785E+00

H 2.854735113869E+01 -3.489323046852E-01 2.742299483857E+00
H 2.286262318744E+01 -8.329812994430E-01 2.635925334146E+00
H 1.717789523619E+01 -1.290257589857E+00 2.444830375349E+00
H 1.149316728494E+01 -1.706063939706E+00 2.175156556675E+00
H 5.808439333687E+00 -2.067035990779E+00 1.835571416545E+00

PBE0/POB-TZVP optimized geometry, *all*-[101.3]-$(SiMe_2)_\infty$

Energy (a.u): -1.033534532589E+04
Unit cell length (Å): 51.06608824

Si	-4.933957213549E-01	-8.286352616699E-04	9.034697275820E-01
Si	-5.964762318229E+00	-2.018487872284E-01	8.806334665386E-01
Si	-1.143612891510E+01	-3.927473981564E-01	8.136385662779E-01
Si	-1.690749551198E+01	-5.639520145705E-01	7.058444308453E-01
Si	-2.237886210885E+01	-7.068777221155E-01	5.626563083004E-01
Si	2.321585953176E+01	-8.143576290093E-01	3.912542490092E-01
Si	1.774449293489E+01	-8.810022439233E-01	2.002330679372E-01
Si	1.227312633802E+01	-9.034697275820E-01	-8.286352616697E-04
Si	6.801759741144E+00	-8.806334665386E-01	-2.018487872284E-01
Si	1.330393144270E+00	-8.136385662779E-01	-3.927473981564E-01
Si	-4.140973452604E+00	-7.058444308453E-01	-5.639520145705E-01
Si	-9.612340049478E+00	-5.626563083004E-01	-7.068777221155E-01
Si	-1.508370664635E+01	-3.912542490092E-01	-8.143576290093E-01
Si	-2.055507324323E+01	-2.002330679372E-01	-8.810022439233E-01
Si	2.503964839739E+01	8.286352616697E-04	-9.034697275820E-01
Si	1.956828180052E+01	2.018487872284E-01	-8.806334665386E-01
Si	1.409691520364E+01	3.927473981564E-01	-8.136385662779E-01
Si	8.625548606768E+00	5.639520145705E-01	-7.058444308453E-01
Si	3.154182009894E+00	7.068777221155E-01	-5.626563083004E-01
Si	-2.317184586980E+00	8.143576290093E-01	-3.912542490092E-01
Si	-7.788551183853E+00	8.810022439233E-01	-2.002330679372E-01
Si	-1.325991778073E+01	9.034697275820E-01	8.286352616697E-04
Si	-1.873128437760E+01	8.806334665386E-01	2.018487872284E-01
Si	-2.420265097447E+01	8.136385662779E-01	3.927473981564E-01
Si	2.139207066614E+01	7.058444308453E-01	5.639520145705E-01
Si	1.592070406927E+01	5.626563083004E-01	7.068777221155E-01
Si	1.044933747239E+01	3.912542490092E-01	8.143576290093E-01
Si	4.977970875519E+00	2.002330679372E-01	8.810022439233E-01
C	2.480757654165E-02	1.410697416816E+00	2.037141751702E+00
C	-5.446559020332E+00	9.220216021069E-01	2.299976061525E+00
C	-1.091792561721E+01	3.871117742409E-01	2.447479967759E+00
C	-1.638929221408E+01	-1.672094544234E-01	2.472257008624E+00
C	-2.186065881095E+01	-7.131461028371E-01	2.373064759830E+00
C	2.373406282966E+01	-1.223322627816E+00	2.154877134923E+00
C	1.826269623279E+01	-1.672156648085E+00	1.828634972487E+00
C	1.279132963591E+01	-2.037141751702E+00	1.410697416816E+00
C	7.319963039040E+00	-2.299976061525E+00	9.220216021069E-01
C	1.848596442166E+00	-2.447479967759E+00	3.871117742409E-01
C	-3.622770154707E+00	-2.472257008624E+00	-1.672094544234E-01
C	-9.094136751581E+00	-2.373064759830E+00	-7.131461028371E-01

C -1.456550334846E+01 -2.154877134923E+00 -1.223322627816E+00
C -2.003686994533E+01 -1.828634972487E+00 -1.672156648085E+00
C 2.555785169529E+01 -1.410697416816E+00 -2.037141751702E+00
C 2.008648509841E+01 -9.220216021069E-01 -2.299976061525E+00
C 1.461511850154E+01 -3.871117742409E-01 -2.447479967759E+00
C 9.143751904665E+00 1.672094544234E-01 -2.472257008624E+00
C 3.672385307791E+00 7.131461028371E-01 -2.373064759830E+00
C -1.798981289083E+00 1.223322627816E+00 -2.154877134923E+00
C -7.270347885957E+00 1.672156648085E+00 -1.828634972487E+00
C -1.274171448283E+01 2.037141751702E+00 -1.410697416816E+00
C -1.821308107970E+01 2.299976061525E+00 -9.220216021069E-01
C -2.368444767658E+01 2.447479967759E+00 -3.871117742409E-01
C 2.191027396404E+01 2.472257008624E+00 1.672094544234E-01
C 1.643890736716E+01 2.373064759830E+00 7.131461028371E-01
C 1.096754077029E+01 2.154877134923E+00 1.223322627816E+00
C 5.496174173416E+00 1.828634972487E+00 1.672156648085E+00
C -1.011615975354E+00 -1.414421911210E+00 2.034553716281E+00
C -6.482982572228E+00 -1.831690193971E+00 1.668804722145E+00
C -1.195434916910E+01 -2.157109881935E+00 1.219374890919E+00
C -1.742571576598E+01 -2.374363073112E+00 7.088005109962E-01
C -2.289708236285E+01 -2.472555785326E+00 1.626839137588E-01
C 2.269763927777E+01 -2.446764225970E+00 -3.915903342234E-01
C 1.722627268089E+01 -2.298281691527E+00 -9.262286077088E-01
C 1.175490608402E+01 -2.034553716281E+00 -1.414421911210E+00
C 6.283539487144E+00 -1.668804722145E+00 -1.831690193971E+00
C 8.121728902706E-01 -1.219374890919E+00 -2.157109881935E+00
C -4.659193706603E+00 -7.088005109962E-01 -2.374363073112E+00
C -1.013056030348E+01 -1.626839137588E-01 -2.472555785326E+00
C -1.560192690035E+01 3.915903342234E-01 -2.446764225970E+00
C -2.107329349722E+01 9.262286077088E-01 -2.298281691527E+00
C 2.452142814339E+01 1.414421911210E+00 -2.034553716281E+00
C 1.905006154652E+01 1.831690193971E+00 -1.668804722145E+00
C 1.357869494964E+01 2.157109881935E+00 -1.219374890919E+00
C 8.107328352769E+00 2.374363073112E+00 -7.088005109962E-01
C 2.635961755895E+00 2.472555785326E+00 -1.626839137588E-01
C -2.835404840979E+00 2.446764225970E+00 3.915903342234E-01
C -8.306771437852E+00 2.298281691527E+00 9.262286077088E-01
C -1.377813803473E+01 2.034553716281E+00 1.414421911210E+00
C -1.924950463160E+01 1.668804722145E+00 1.831690193971E+00
C -2.472087122847E+01 1.219374890919E+00 2.157109881935E+00
C 2.087385041214E+01 7.088005109962E-01 2.374363073112E+00
C 1.540248381527E+01 1.626839137588E-01 2.472555785326E+00
C 9.931117218394E+00 -3.915903342234E-01 2.446764225970E+00
C 4.459750621520E+00 -9.262286077088E-01 2.298281691527E+00
H -7.745452728497E-01 1.629576182311E+00 2.747295443019E+00

H -6.245911869723E+00 9.773885573270E-01 3.041029824450E+00
H -1.171727846660E+01 2.761905888597E-01 3.182274272248E+00
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H -2.266001166034E+01 -1.131897937970E+00 2.986964653826E+00
H 2.293470998027E+01 -1.768181057932E+00 2.660204227415E+00
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H 1.199197678652E+01 -2.747295443019E+00 1.629576182311E+00
H 6.520610189649E+00 -3.041029824450E+00 9.773885573270E-01
H 1.049243592775E+00 -3.182274272248E+00 2.761905888597E-01
H -4.422123004099E+00 -3.163946200016E+00 -4.388567290045E-01
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H -1.536485619785E+01 -2.660204227415E+00 -1.768181057932E+00
H -2.083622279472E+01 -2.200050052996E+00 -2.315800196368E+00
H 2.475849884589E+01 -1.629576182311E+00 -2.747295443019E+00
H 1.928713224902E+01 -9.773885573270E-01 -3.041029824450E+00
H 1.381576565215E+01 -2.761905888597E-01 -3.182274272248E+00
H 8.344399055273E+00 4.388567290045E-01 -3.163946200016E+00
H 2.873032458400E+00 1.131897937970E+00 -2.986964653826E+00
H -2.598334138474E+00 1.768181057932E+00 -2.660204227415E+00
H -8.069700735348E+00 2.315800196368E+00 -2.200050052996E+00
H -1.354106733222E+01 2.747295443019E+00 -1.629576182311E+00
H -1.901243392910E+01 3.041029824450E+00 -9.773885573270E-01
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H -2.164429139434E+01 2.872665908653E-01 2.743042686271E+00
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H 1.483148591816E+01 -1.448979872437E+00 -2.346755761090E+00
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H -1.582613872465E+00 3.303202027592E-01 -2.738191709246E+00
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H -1.799671366309E+01 1.965489340061E+00 -1.934853205553E+00
H -2.346808025996E+01 2.346755761090E+00 -1.448979872437E+00
H 2.212664138065E+01 2.610346049058E+00 -8.904486381031E-01
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H 9.124538865856E-01 1.142444398206E+00 2.613511518715E+00
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H -1.550164590404E+01 -7.362987814719E-01 2.755628016596E+00
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H -2.311346681759E+01 -2.608708883227E+00 -8.952211377661E-01
H 2.248125482303E+01 -2.344097661341E+00 -1.453268411899E+00
H 1.700988822616E+01 -1.961943594617E+00 -1.938442739539E+00
H 1.153852162928E+01 -1.481409483695E+00 -2.326415453987E+00
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H -1.034694475821E+01 8.952211377661E-01 -2.608708883227E+00
H -1.581831135509E+01 1.453268411899E+00 -2.344097661341E+00
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H 1.336231049491E+01 2.738787383799E+00 -3.253099895083E-01
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H -1.399452248946E+01 1.481409483695E+00 2.326415453987E+00
H -1.946588908634E+01 9.265913154339E-01 2.597731983306E+00
H -2.493725568321E+01 3.253099895083E-01 2.738787383799E+00
H 2.065746595740E+01 -2.922837376676E-01 2.742508548688E+00
H 1.518609936053E+01 -8.952211377661E-01 2.608708883227E+00
H 9.714732763657E+00 -1.453268411899E+00 2.344097661341E+00
H 4.243366166783E+00 -1.938442739539E+00 1.961943594617E+00

PBE0/POB-TZVP optimized geometry, *all*-[86.9]-$(SiMe_2)_\infty$

Energy (a.u): -8.858896067459E+03
Unit cell length (Å): 41.44111002

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Si	1.117196623864E+01	-2.633827790019E-01	9.902439051814E-01
Si	-1.818215336043E+01	-5.107022103954E-01	8.883336829823E-01
Si	-6.095162937283E+00	-7.232181301257E-01	7.258849883288E-01
Si	5.991827485860E+00	-8.864479294625E-01	5.139684313024E-01
Si	1.807881790900E+01	-9.892677673308E-01	2.670257750557E-01
Si	-1.127530169006E+01	-1.024670641698E+00	1.885753519872E-03
Si	8.116887330844E-01	-9.902439051814E-01	-2.633827790019E-01
Si	1.289867915623E+01	-8.883336829823E-01	-5.107022103954E-01
Si	-1.645544044283E+01	-7.258849883288E-01	-7.232181301257E-01
Si	-4.368450019691E+00	-5.139684313024E-01	-8.864479294625E-01
Si	7.718540403452E+00	-2.670257750557E-01	-9.892677673308E-01
Si	1.980553082659E+01	-1.885753519872E-03	-1.024670641698E+00
Si	-9.548588772467E+00	2.633827790019E-01	-9.902439051814E-01
Si	2.538401650676E+00	5.107022103954E-01	-8.883336829823E-01
Si	1.462539207382E+01	7.232181301257E-01	-7.258849883288E-01
Si	-1.472872752524E+01	8.864479294625E-01	-5.139684313024E-01
Si	-2.641737102099E+00	9.892677673308E-01	-2.670257750557E-01
Si	9.445253321044E+00	1.024670641698E+00	-1.885753519872E-03
Si	-1.990886627802E+01	9.902439051814E-01	2.633827790019E-01
Si	-7.821875854875E+00	8.883336829823E-01	5.107022103954E-01
Si	4.265114568268E+00	7.258849883288E-01	7.232181301257E-01
Si	1.635210499141E+01	5.139684313024E-01	8.864479294625E-01
Si	-1.300201460765E+01	2.670257750557E-01	9.892677673308E-01
C	-2.248931366820E-01	1.341467076803E+00	2.153505942875E+00
C	1.186209728646E+01	7.383893428430E-01	2.427324235144E+00
C	-1.749202231260E+01	8.499159541448E-02	2.535724392132E+00
C	-5.405031889457E+00	-5.741981887863E-01	2.471319122278E+00
C	6.681958533685E+00	-1.194257315329E+00	2.238497538289E+00
C	1.876894895683E+01	-1.732929779435E+00	1.853126046358E+00
C	-1.058517064223E+01	-2.153505942875E+00	1.341467076803E+00
C	1.501819780910E+00	-2.427324235144E+00	7.383893428430E-01
C	1.358881020405E+01	-2.535724392132E+00	8.499159541448E-02
C	-1.576530939501E+01	-2.471319122278E+00	-5.741981887863E-01
C	-3.678318971866E+00	-2.238497538289E+00	-1.194257315329E+00
C	8.408671451277E+00	-1.853126046358E+00	-1.732929779435E+00
C	2.049566187442E+01	-1.341467076803E+00	-2.153505942875E+00
C	-8.858457724641E+00	-7.383893428430E-01	-2.427324235144E+00
C	3.228532698502E+00	-8.499159541448E-02	-2.535724392132E+00
C	1.531552312164E+01	5.741981887863E-01	-2.471319122278E+00

C -1.403859647742E+01 1.194257315329E+00 -2.238497538289E+00
C -1.951606054274E+00 1.732929779435E+00 -1.853126046358E+00
C 1.013538436887E+01 2.153505942875E+00 -1.341467076803E+00
C -1.921873523019E+01 2.427324235144E+00 -7.383893428430E-01
C -7.131744807049E+00 2.535724392132E+00 -8.499159541448E-02
C 4.955245616094E+00 2.471319122278E+00 5.741981887863E-01
C 1.704223603924E+01 2.238497538289E+00 1.194257315329E+00
C -1.231188355982E+01 1.853126046358E+00 1.732929779435E+00
C -1.609127008338E+00 -1.335419848809E+00 2.153808980847E+00
C 1.047786341480E+01 -1.847363304660E+00 1.734787629414E+00
C -1.887625618426E+01 -2.233412004210E+00 1.197543367909E+00
C -6.789265761114E+00 -2.467257366561E+00 5.786885049139E-01
C 5.297724662029E+00 -2.532963216717E+00 -7.960302336262E-02
C 1.738471508517E+01 -2.426051809573E+00 -7.324697371472E-01
C -1.196940451389E+01 -2.153808980847E+00 -1.335419848809E+00
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C 1.220457633240E+01 -1.197543367909E+00 -2.233412004210E+00
C -1.714954326666E+01 -5.786885049139E-01 -2.467257366561E+00
C -5.062552843522E+00 7.960302336262E-02 -2.532963216717E+00
C 7.024437579621E+00 7.324697371472E-01 -2.426051809573E+00
C 1.911142800276E+01 1.335419848809E+00 -2.153808980847E+00
C -1.024269159630E+01 1.847363304660E+00 -1.734787629414E+00
C 1.844298826845E+00 2.233412004210E+00 -1.197543367909E+00
C 1.393128924999E+01 2.467257366561E+00 -5.786885049139E-01
C -1.542283034907E+01 2.532963216717E+00 7.960302336262E-02
C -3.335839925930E+00 2.426051809573E+00 7.324697371472E-01
C 8.751150497213E+00 2.153808980847E+00 1.335419848809E+00
C -2.060296910185E+01 1.734787629414E+00 1.847363304660E+00
C -8.515978678706E+00 1.197543367909E+00 2.233412004210E+00
C 3.571011744437E+00 5.786885049139E-01 2.467257366561E+00
C 1.565800216758E+01 -7.960302336262E-02 2.532963216717E+00
C -1.369611743148E+01 -7.324697371472E-01 2.426051809573E+00
H -1.017112704330E+00 1.754172108485E+00 2.780461930803E+00
H 1.106987771881E+01 9.747636414671E-01 3.139733138040E+00
H -1.828424188025E+01 1.289266431564E-01 3.285036720573E+00
H -6.197251457106E+00 -7.256964928240E-01 3.206470479380E+00
H 5.889738966037E+00 -1.530864612089E+00 2.909388573959E+00
H 1.797672938918E+01 -2.231706837913E+00 2.414036645216E+00
H -1.137739020988E+01 -2.780461930803E+00 1.754172108485E+00
H 7.096002132618E-01 -3.139733138040E+00 9.747636414671E-01
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H -4.470538539514E+00 -2.909388573959E+00 -1.530864612089E+00
H 7.616451883629E+00 -2.414036645216E+00 -2.231706837913E+00
H 1.970344230677E+01 -1.754172108485E+00 -2.780461930803E+00

H -9.650677292289E+00 -9.747636414671E-01 -3.139733138040E+00
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H -1.483081604506E+01 1.530864612089E+00 -2.909388573959E+00
H -2.743825621922E+00 2.231706837913E+00 -2.414036645216E+00
H 9.343164801221E+00 2.780461930803E+00 -1.754172108485E+00
H 2.143015522436E+01 3.139733138040E+00 -9.747636414671E-01
H -7.923964374697E+00 3.285036720573E+00 -1.289266431564E-01
H 4.163026048445E+00 3.206470479380E+00 7.256964928240E-01
H 1.625001647159E+01 2.909388573959E+00 1.530864612089E+00
H -1.310410312747E+01 2.414036645216E+00 2.231706837913E+00
H 2.198058216633E-01 2.164589145387E+00 1.594451790901E+00
H 1.230679624481E+01 1.678158068851E+00 2.100359059253E+00
H -1.704732335425E+01 1.077363293210E+00 2.463130328724E+00
H -4.960332931112E+00 4.031479895644E-01 2.658043336807E+00
H 7.126657492031E+00 -2.985411833368E-01 2.671815084112E+00
H 1.921364791517E+01 -9.798852679562E-01 2.503507048817E+00
H -1.014047168389E+01 -1.594451790901E+00 2.164589145387E+00
H 1.946518739255E+00 -2.100359059253E+00 1.678158068851E+00
H 1.403350916240E+01 -2.463130328724E+00 1.077363293210E+00
H -1.532061043666E+01 -2.658043336807E+00 4.031479895644E-01
H -3.233620013520E+00 -2.671815084112E+00 -2.985411833368E-01
H 8.853370409623E+00 -2.503507048817E+00 -9.798852679562E-01
H 2.094036083277E+01 -2.164589145387E+00 -1.594451790901E+00
H -8.413758766296E+00 -1.678158068851E+00 -2.100359059253E+00
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H -1.359389751907E+01 2.985411833368E-01 -2.671815084112E+00
H -1.506907095928E+00 9.798852679562E-01 -2.503507048817E+00
H 1.058008332721E+01 1.594451790901E+00 -2.164589145387E+00
H -1.877403627185E+01 2.100359059253E+00 -1.678158068851E+00
H -6.687045848704E+00 2.463130328724E+00 -1.077363293210E+00
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H 1.748693499758E+01 2.671815084112E+00 2.985411833368E-01
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H 5.392006363582E-01 9.277991462710E-01 2.813059014651E+00
H 1.262619105950E+01 1.681119090032E-01 2.957338442211E+00
H -1.672792853956E+01 -6.030318770451E-01 2.900080142168E+00
H -4.640938116417E+00 -1.333080037230E+00 2.645186173045E+00
H 7.446052306726E+00 -1.972280995897E+00 2.210027137605E+00
H 1.953304272987E+01 -2.477074264041E+00 1.624258404981E+00
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H 2.265913553950E+00 -2.957338442211E+00 1.681119090032E-01
H 1.435290397709E+01 -2.900080142168E+00 -6.030318770451E-01
H -1.500121562197E+01 -2.645186173045E+00 -1.333080037230E+00

H -2.914225198825E+00 -2.210027137605E+00 -1.972280995897E+00
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H -1.187512281234E+00 2.477074264041E+00 -1.624258404981E+00
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H 1.780632981228E+01 2.210027137605E+00 1.972280995897E+00
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H 9.711420759490E+00 -1.616290596453E+00 2.475821803664E+00
H -1.964269883957E+01 -2.202006664971E+00 1.973133432666E+00
H -7.555708416428E+00 -2.637659618259E+00 1.335979278990E+00
H 4.531282006715E+00 -2.893560427500E+00 6.077803452599E-01
H 1.661827242986E+01 -2.952269875443E+00 -1.618378145947E-01
H -1.273584716920E+01 -2.809787010231E+00 -9.204269948343E-01
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H -1.791598592198E+01 -1.335979278990E+00 -2.637659618259E+00
H -5.828995498836E+00 -6.077803452599E-01 -2.893560427500E+00
H 6.257994924306E+00 1.618378145947E-01 -2.952269875443E+00
H 1.834498534745E+01 9.204269948343E-01 -2.809787010231E+00
H -1.100913425161E+01 1.616290596453E+00 -2.475821803664E+00
H 1.077856171531E+00 2.202006664971E+00 -1.973133432666E+00
H 1.316484659467E+01 2.637659618259E+00 -1.335979278990E+00
H -1.618927300439E+01 2.893560427500E+00 -6.077803452599E-01
H -4.102282581245E+00 2.952269875443E+00 1.618378145947E-01
H 7.984707841898E+00 2.809787010231E+00 9.204269948343E-01
H 2.007169826504E+01 2.475821803664E+00 1.616290596453E+00
H -9.282421334020E+00 1.973133432666E+00 2.202006664971E+00
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H 1.489155951227E+01 6.077803452599E-01 2.893560427500E+00
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H -8.192099037513E-01 -1.747032549605E+00 2.784365537917E+00
H 1.126778051939E+01 -2.408150688772E+00 2.237325286652E+00
H -1.808633907967E+01 -2.905157338155E+00 1.537815014455E+00
H -5.999348656527E+00 -3.204182315943E+00 7.335051903838E-01
H 6.087641766616E+00 -3.284847564061E+00 -1.207918002380E-01
H 1.817463218976E+01 -3.141655879155E+00 -9.668570292914E-01
H -1.117948740930E+01 -2.784365537917E+00 -1.747032549605E+00

H 9.075030138405E-01 -2.237325286652E+00 -2.408150688772E+00
H 1.299449343698E+01 -1.537815014455E+00 -2.905157338155E+00
H -1.635962616208E+01 -7.335051903838E-01 -3.204182315943E+00
H -4.272635738935E+00 1.207918002380E-01 -3.284847564061E+00
H 7.814354684208E+00 9.668570292914E-01 -3.141655879155E+00
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H -7.726061574119E+00 1.537815014455E+00 2.905157338155E+00
H 4.360928849024E+00 7.335051903838E-01 3.204182315943E+00
H 1.644791927217E+01 -1.207918002380E-01 3.284847564061E+00
H -1.290620032689E+01 -9.668570292914E-01 3.141655879155E+00
H -2.051966343101E+00 -2.159485759614E+00 1.594656568726E+00
H 1.003502408004E+01 -2.498630557099E+00 9.814039215783E-01
H -1.931909551902E+01 -2.667497811300E+00 3.012702190215E-01
H -7.232105095877E+00 -2.654579497909E+00 -3.993945510890E-01
H 4.854885327266E+00 -2.460755978636E+00 -1.072841242573E+00
H 1.694187575041E+01 -2.099236006010E+00 -1.673175576331E+00
H -1.241224384865E+01 -1.594656568726E+00 -2.159485759614E+00
H -3.252534255094E-01 -9.814039215783E-01 -2.498630557099E+00
H 1.176173699763E+01 -3.012702190215E-01 -2.667497811300E+00
H -1.759238260143E+01 3.993945510890E-01 -2.654579497909E+00
H -5.505392178285E+00 1.072841242573E+00 -2.460755978636E+00
H 6.581598244858E+00 1.673175576331E+00 -2.099236006010E+00
H 1.866858866800E+01 2.159485759614E+00 -1.594656568726E+00
H -1.068553093106E+01 2.498630557099E+00 -9.814039215783E-01
H 1.401459492082E+00 2.667497811300E+00 -3.012702190215E-01
H 1.348844991523E+01 2.654579497909E+00 3.993945510890E-01
H -1.586566968384E+01 2.460755978636E+00 1.072841242573E+00
H -3.778679260693E+00 2.099236006010E+00 1.673175576331E+00
H 8.308311162450E+00 1.594656568726E+00 2.159485759614E+00
H -2.104580843661E+01 9.814039215783E-01 2.498630557099E+00
H -8.958818013469E+00 3.012702190215E-01 2.667497811300E+00
H 3.128172409674E+00 -3.993945510890E-01 2.654579497909E+00
H 1.521516283282E+01 -1.072841242573E+00 2.460755978636E+00
H -1.413895676624E+01 -1.673175576331E+00 2.099236006010E+00

PBE0/POB-TZVP optimized geometry, *all*-[76.7]-$(SiMe_2)_\infty$

Energy (a.u): -7.013282449815E+03
Unit cell length (Å): 32.79660496

Si	-5.482182835171E-01	-1.011925901488E-03	1.100946595249E+00
Si	-7.452766695943E+00	-3.584338720651E-01	1.040965700175E+00
Si	-1.435731510837E+01	-6.770139465158E-01	8.681800192402E-01
Si	1.153474143823E+01	-9.222290549079E-01	6.013135620195E-01
Si	4.630193025802E+00	-1.067506335342E+00	2.692854500127E-01
Si	-2.274355386623E+00	-1.097102740275E+00	-9.192391889717E-02
Si	-9.178903799049E+00	-1.007811039996E+00	-4.431719048480E-01
Si	-1.608345221147E+01	-8.093073757341E-01	-7.463953383879E-01
Si	9.808604335121E+00	-5.231026996134E-01	-9.687352554966E-01
Si	2.904055922696E+00	-1.802117292149E-01	-1.086097676196E+00
Si	-4.000492489730E+00	1.822079783172E-01	-1.085764561138E+00
Si	-1.090504090216E+01	5.248826241504E-01	-9.677720085071E-01
Si	1.498701564444E+01	8.106780932639E-01	-7.449063422248E-01
Si	8.082467232015E+00	1.008624012006E+00	-4.413185153497E-01
Si	1.177918819589E+00	1.097269868632E+00	-8.990697957418E-02
Si	-5.726629592836E+00	1.067009509097E+00	2.712473724888E-01
Si	-1.263117800526E+01	9.211221128919E-01	6.030078629059E-01
Si	1.326087854133E+01	6.754168430731E-01	8.694230947462E-01
Si	6.356330128908E+00	3.565196781352E-01	1.041622843781E+00
C	-1.284615431500E+00	1.329372576104E+00	2.210770483406E+00
C	-8.189163843925E+00	5.395075006275E-01	2.522631410484E+00
C	-1.509371225635E+01	-3.088215838631E-01	2.561126081577E+00
C	1.079834429024E+01	-1.123685057881E+00	2.322083001766E+00
C	3.893795877819E+00	-1.816779820108E+00	1.831406197883E+00
C	-3.010752534606E+00	-2.312998298583E+00	1.142268115264E+00
C	-9.915300947032E+00	-2.558567521540E+00	3.293475582404E-01
C	1.597675559956E+01	-2.526876253272E+00	-5.192629170725E-01
C	9.072207187139E+00	-2.221358734437E+00	-1.311603198126E+00
C	2.167658774713E+00	-1.675122528794E+00	-1.961810921042E+00
C	-4.736889637713E+00	-9.473608049524E-01	-2.399425990031E+00
C	-1.164143805014E+01	-1.169378380765E-01	-2.577026022069E+00
C	1.425061849646E+01	7.261571580326E-01	-2.475365297938E+00
C	7.346070084032E+00	1.490561758580E+00	-2.105460334524E+00
C	4.415216716066E-01	2.093440864136E+00	-1.507396074282E+00
C	-6.463026740819E+00	2.469463168981E+00	-7.459820597319E-01
C	-1.336757515324E+01	2.577880821798E+00	9.627068609491E-02
C	1.252448139335E+01	2.406945087631E+00	9.280910092897E-01
C	5.619932980926E+00	1.975179505618E+00	1.659338270812E+00
C	1.881697796963E-01	-1.333421104951E+00	2.208345681558E+00
C	-6.716378632729E+00	-1.978221342132E+00	1.655730296249E+00

C -1.362092704515E+01 -2.408650601627E+00 9.236908420387E-01
C 1.227112950144E+01 -2.578065194371E+00 9.155515255337E-02
C 5.366581089015E+00 -2.468106420501E+00 -7.505019583357E-01
C -1.537967323410E+00 -2.090690019353E+00 -1.511230536801E+00
C -8.442515735836E+00 -1.486714914210E+00 -2.108193837447E+00
C -1.534706414826E+01 -7.216311793541E-01 -2.476701623807E+00
C 1.054499239833E+01 1.216524910466E-01 -2.576820359242E+00
C 3.640443985909E+00 9.517532264095E-01 -2.397700625266E+00
C -3.264104426516E+00 1.678716731718E+00 -1.958752824384E+00
C -1.016865283894E+01 2.223765231171E+00 -1.307543761799E+00
C 1.572340370765E+01 2.527834262554E+00 -5.146420439902E-01
C 8.818855295228E+00 2.557973228199E+00 3.340291247787E-01
C 1.914306882803E+00 2.310916103525E+00 1.146503054882E+00
C -4.990241529623E+00 1.813435361476E+00 1.834735589161E+00
C -1.189478994205E+01 1.119440759662E+00 2.324146053498E+00
C 1.399726660455E+01 3.041373816257E-01 2.561699230097E+00
C 7.092718192122E+00 -5.441240008874E-01 2.521652546257E+00
H -2.104116646164E+00 9.321432603846E-01 2.811227135958E+00
H -9.008665058590E+00 -3.116679145262E-02 2.961573517396E+00
H -1.591321347102E+01 -9.910994378334E-01 2.790987454675E+00
H 9.978843075580E+00 -1.843631081633E+00 2.317954594608E+00
H 3.074294663155E+00 -2.496376690853E+00 1.593735387445E+00
H -3.830253749271E+00 -2.878601150345E+00 6.968102216985E-01
H -1.073480216170E+01 -2.948884509097E+00 -2.756251436932E-01
H 1.515725438490E+01 -2.699610474631E+00 -1.218192248001E+00
H 8.252705972474E+00 -2.157791756467E+00 -2.028749320038E+00
H 1.348157560048E+00 -1.382142819900E+00 -2.619459923959E+00
H -5.556390852377E+00 -4.567172626419E-01 -2.926311400011E+00
H -1.246093926480E+01 5.182006967221E-01 -2.916051629472E+00
H 1.343111728179E+01 1.436963569884E+00 -2.589792417676E+00
H 6.526568869367E+00 2.200009143462E+00 -1.982889012656E+00
H -3.779795430580E-01 2.724649589687E+00 -1.161108815421E+00
H -7.282527955484E+00 2.954031975574E+00 -2.135044615763E-01
H -1.418707636791E+01 2.863299160380E+00 7.572364135438E-01
H 1.170498017869E+01 2.462283452494E+00 1.645918973523E+00
H 4.800431766261E+00 1.794441126266E+00 2.356240673656E+00
H -1.673329503812E+00 2.164788286620E+00 1.627646044053E+00
H -8.577877916237E+00 1.518998279560E+00 2.242361299457E+00
H -1.548242632866E+01 7.086012392224E-01 2.614081914245E+00
H 1.040963021793E+01 -1.785837404659E-01 2.702526191964E+00
H 3.505081805507E+00 -1.046416400863E+00 2.498109822769E+00
H -3.399466606918E+00 -1.800853607402E+00 2.022984492110E+00
H -1.030401501934E+01 -2.360140382457E+00 1.328637401891E+00
H 1.558804152725E+01 -2.663669325722E+00 4.903118332449E-01
H 8.683493114826E+00 -2.678548366456E+00 -4.011466305057E-01

H 1.778944702401E+00 -2.403165129725E+00 -1.249134632410E+00
H -5.125603710025E+00 -1.867361662239E+00 -1.961759514571E+00
H -1.203015212245E+01 -1.129200583548E+00 -2.461797313494E+00
H 1.386190442415E+01 -2.686731002767E-01 -2.695061174778E+00
H 6.957356011720E+00 6.209692823018E-01 -2.636273339593E+00
H 5.280759929442E-02 1.443320007812E+00 -2.291804382067E+00
H -6.851740813131E+00 2.109264615058E+00 -1.698982858735E+00
H -1.375628922556E+01 2.546637672650E+00 -9.220501802237E-01
H 1.213576732104E+01 2.708043023255E+00 -4.519905760273E-02
H 5.231218908614E+00 2.575989892674E+00 8.365500842452E-01
H -5.308041667030E-01 1.721333516705E+00 2.895272672890E+00
H -7.435352579128E+00 6.879734187264E-01 3.297314892642E+00
H -1.433990099155E+01 -4.199392741786E-01 3.342041880665E+00
H 1.155215555504E+01 -1.482345030697E+00 3.024606773795E+00
H 4.647607142616E+00 -2.384115702186E+00 2.379408591374E+00
H -2.256941269809E+00 -3.027530443977E+00 1.476364567750E+00
H -9.161489682235E+00 -3.342865285188E+00 4.133335350529E-01
H -1.606603809466E+01 -3.295948802850E+00 -6.944885996973E-01
H 9.826018451935E+00 -2.891865125807E+00 -1.727052118569E+00
H 2.921470039510E+00 -2.174402990473E+00 -2.572462742420E+00
H -3.983078372916E+00 -1.221310551782E+00 -3.139107112257E+00
H -1.088762678534E+01 -1.358701642203E-01 -3.365580518215E+00
H 1.500442976125E+01 9.642938638778E-01 -3.227341052663E+00
H 8.099881348829E+00 1.959961689264E+00 -2.739369106698E+00
H 1.195332936403E+00 2.743237253679E+00 -1.954544012332E+00
H -5.709215476022E+00 3.229240495947E+00 -9.579137463541E-01
H -1.261376388845E+01 3.365305423649E+00 1.425213376044E-01
H 1.327829265815E+01 3.136687290606E+00 1.227512023187E+00
H 6.373744245723E+00 2.568160418907E+00 2.179482734246E+00
H -5.656443788063E-01 -1.726630156245E+00 2.892128427516E+00
H -7.470192791232E+00 -2.572149137103E+00 2.174789036712E+00
H -1.437474120366E+01 -3.138935847950E+00 1.221777508451E+00
H 1.151731534294E+01 -3.365570154063E+00 1.363674293179E-01
H 4.612766930513E+00 -3.227492711782E+00 -9.638201767402E-01
H -2.291781481913E+00 -2.739666354471E+00 -1.959562911438E+00
H -9.196329894338E+00 -1.954954637349E+00 -2.742956598929E+00
H 1.669572665226E+01 -9.583932510230E-01 -3.229108377570E+00
H 9.791178239832E+00 1.420249150543E-01 -3.365336158722E+00
H 2.886629827406E+00 1.227052477842E+00 -3.136877548506E+00
H -4.017918585019E+00 2.179109864974E+00 -2.568489582239E+00
H -1.092246699744E+01 2.895026885864E+00 -1.721765915514E+00
H 1.496958954915E+01 3.297222822699E+00 -6.884621958928E-01
H 8.065041136726E+00 3.342113505011E+00 4.194470852454E-01
H 1.160492724300E+00 3.024834330822E+00 1.481902766305E+00
H -5.744055688126E+00 2.379767421747E+00 2.383771288545E+00

H -1.264860410055E+01 1.476815786630E+00 3.027321203649E+00
H 1.324345244604E+01 4.138282458732E-01 3.342813892609E+00
H 6.338904033619E+00 -6.940040065305E-01 3.296060827203E+00
H 1.007668224384E+00 -9.372886988823E-01 2.809530091663E+00
H -5.896880188042E+00 -1.798756741332E+00 2.352964858753E+00
H -1.280142860047E+01 -2.465301580271E+00 1.641419373386E+00
H 1.309062794613E+01 -2.864692739893E+00 7.520006296662E-01
H 6.186079533703E+00 -2.953649990860E+00 -2.189090507698E-01
H -7.184688787225E-01 -2.722533434715E+00 -1.166096538831E+00
H -7.623017291148E+00 -2.196388136460E+00 -1.986919373058E+00
H -1.452756570357E+01 -1.432230103146E+00 -2.592428662983E+00
H 1.136449084302E+01 -5.128677148168E-01 -2.917008081599E+00
H 4.459942430597E+00 4.620718483755E-01 -2.925484412529E+00
H -2.444605981829E+00 1.386938757013E+00 -2.616939113795E+00
H -9.349154394254E+00 2.161509330756E+00 -2.024807856086E+00
H 1.654290215234E+01 2.701846829238E+00 -1.213257249040E+00
H 9.638353739916E+00 2.949397300300E+00 -2.702313934343E-01
H 2.733805327490E+00 2.877334809260E+00 7.020782267222E-01
H -4.170743084935E+00 2.493468445186E+00 1.598306777147E+00
H -1.107529149736E+01 1.839396084928E+00 2.321333987983E+00
H 1.481676504924E+01 9.859966176963E-01 2.792808642014E+00
H 7.912216636809E+00 2.574911762358E-02 2.961639144791E+00
H 5.768871911119E-01 -2.167772238980E+00 1.623700852089E+00
H -6.327661221314E+00 -2.577531164528E+00 8.318497659165E-01
H -1.323220963374E+01 -2.707974593883E+00 -5.014514987235E-02
H 1.265984691286E+01 -2.544966957435E+00 -9.267060605904E-01
H 5.755298500431E+00 -2.106172661918E+00 -1.702843990317E+00
H -1.149249911994E+00 -1.439141877846E+00 -2.294452351347E+00
H -8.053798324420E+00 -6.161577407224E-01 -2.637421198011E+00
H -1.495834673685E+01 2.735966482808E-01 -2.694584534064E+00
H 1.093370980975E+01 1.133702595153E+00 -2.459747825065E+00
H 4.029161397325E+00 1.870954274633E+00 -1.958359272300E+00
H -2.875387015101E+00 2.405459027609E+00 -1.244752105306E+00
H -9.779935427526E+00 2.679294970401E+00 -3.962567333833E-01
H 1.611212111907E+01 2.662787729606E+00 4.951792041582E-01
H 9.207572706644E+00 2.357726120899E+00 1.332954791432E+00
H 2.303024294218E+00 1.797168303102E+00 2.026284044130E+00
H -4.601524118207E+00 1.041859413725E+00 2.500033979610E+00
H -1.150607253063E+01 1.736488907563E-01 2.702866441375E+00
H 1.438598401596E+01 -7.133791839660E-01 2.612801384923E+00
H 7.481435603537E+00 -1.523101554887E+00 2.239598756624E+00

PBE0/POB-TZVP optimized geometry, *all*-[61.5]-$(SiMe_2)_\infty$

Energy (a.u): -4.798564791821E+03
Unit cell length (Å): 20.61093641

Si	-9.169336707966E-01	2.041112760861E-03	1.317841513258E+00
Si	-7.258760260022E+00	-6.106241726992E-01	1.167839261167E+00
Si	7.010349565735E+00	-1.083402819013E+00	7.502991083316E-01
Si	6.685229765096E-01	-1.307986935910E+00	1.608744718616E-01
Si	-5.673303612715E+00	-1.232927008742E+00	-4.654045673644E-01
Si	8.595806213041E+00	-8.754183622517E-01	-9.850650289402E-01
Si	2.253979623816E+00	-3.173619189047E-01	-1.279058963706E+00
Si	-4.087846965409E+00	3.133983154375E-01	-1.280035904219E+00
Si	1.018126286035E+01	8.723627725722E-01	-9.877720451797E-01
Si	3.839436271122E+00	1.231479431622E+00	-4.692215145335E-01
Si	-2.502390318103E+00	1.308478993823E+00	1.568220103601E-01
Si	-8.844216907328E+00	1.085721787420E+00	7.469395025902E-01
Si	5.424892918428E+00	6.142388038855E-01	1.165942156374E+00
C	-2.348413940702E-02	1.234766406906E+00	2.426635254163E+00
C	-6.365310728632E+00	-3.438227743850E-02	2.722503369212E+00
C	7.903799097124E+00	-1.295654396373E+00	2.394678772096E+00
C	1.561972507899E+00	-2.260107707427E+00	1.518262127301E+00
C	-4.779854081326E+00	-2.706797579960E+00	2.940299261838E-01
C	9.489255744431E+00	-2.533392747371E+00	-9.975609875777E-01
C	3.147429155206E+00	-1.779618167052E+00	-2.060622700998E+00
C	-3.194397434020E+00	-6.181545113846E-01	-2.651620586816E+00
C	1.107471239174E+01	6.849208932714E-01	-2.635164151686E+00
C	4.732885802512E+00	1.831089175470E+00	-2.015023366575E+00
C	-1.608940786713E+00	2.557776994586E+00	-9.332650118467E-01
C	-7.950767375938E+00	2.698508928796E+00	3.622931100336E-01
C	6.318342449818E+00	2.221044987977E+00	1.574854246510E+00
C	-1.810422661728E+00	-1.227290881322E+00	2.430366780455E+00
C	-8.152249250953E+00	-2.216159865539E+00	1.581632398913E+00
C	6.116860574804E+00	-2.697333332183E+00	3.705650955165E-01
C	-2.249660144216E-01	-2.560580238813E+00	-9.253942054694E-01
C	-6.566792603647E+00	-1.837229071069E+00	-2.009356846191E+00
C	7.702317222110E+00	-6.929908641536E-01	-2.633000048826E+00
C	1.360490632885E+00	6.100031982944E-01	-2.653454671365E+00
C	-4.981335956340E+00	1.773252879349E+00	-2.066034806290E+00
C	9.287773869416E+00	2.530271695758E+00	-1.005311265512E+00
C	2.945947280191E+00	2.707635759749E+00	2.857169708808E-01
C	-3.395879309034E+00	2.264713101729E+00	1.511290892507E+00
C	-9.737705898259E+00	1.302971964855E+00	2.390646283690E+00
C	4.531403927497E+00	4.273565334693E-02	2.722333421690E+00
H	-2.704139977656E+00	2.933166726918E+00	2.026561790166E+00

H -9.045966566882E+00 1.655399929126E+00 3.157541893928E+00
H 5.223143258875E+00 -1.599042696765E-03 3.565167202295E+00
H -1.118683330350E+00 -1.658231693108E+00 3.156055669539E+00
H -7.460509919575E+00 -2.934983446487E+00 2.023929817486E+00
H 6.808599906181E+00 -3.539365862660E+00 4.281460352447E-01
H 4.667733169561E-01 -3.332922213680E+00 -1.265720843952E+00
H -5.875053272269E+00 -2.362946251614E+00 -2.669626331389E+00
H 8.394056553488E+00 -8.516477798913E-01 -3.461952598789E+00
H 2.052229964262E+00 8.547529347356E-01 -3.461187246859E+00
H -4.289596624963E+00 2.365340052904E+00 -2.667505608501E+00
H -1.063142321419E+01 3.334056270390E+00 -1.262730582163E+00
H 3.637686611569E+00 3.538980376064E+00 4.313208029950E-01
H 4.093234933168E-01 2.050038085044E+00 1.847808841373E+00
H -5.932503095908E+00 9.564989891274E-01 2.588853674542E+00
H 8.336606729848E+00 -3.561624981361E-01 2.736823329941E+00
H 1.994780140623E+00 -1.587231449300E+00 2.257819742748E+00
H -4.347046448602E+00 -2.454684803642E+00 1.261576862169E+00
H 9.922063377155E+00 -2.759799451628E+00 -2.367807388419E-02
H 3.580236787929E+00 -2.432677304435E+00 -1.303508648562E+00
H -2.761589801296E+00 -1.548258103736E+00 -2.284721100836E+00
H 1.150752002446E+01 -3.091516300033E-01 -2.742531482783E+00
H 5.165693435236E+00 1.000777756482E+00 -2.572060953112E+00
H -1.176133153989E+00 2.081441019637E+00 -1.812362255777E+00
H -7.517959743215E+00 2.685271229276E+00 -6.374732069766E-01
H 6.751150082542E+00 2.673938161315E+00 6.834532711571E-01
H 7.808253151599E-01 7.528810488566E-01 2.986002971910E+00
H -5.561001274065E+00 -7.210217115278E-01 2.993855593292E+00
H 8.708108551691E+00 -2.029747087055E+00 2.315851978122E+00
H 2.366281962466E+00 -2.873481866042E+00 1.107314583807E+00
H -3.975544626759E+00 -3.058936578729E+00 -3.548952370717E-01
H 1.029356519900E+01 -2.543625785411E+00 -1.735802836088E+00
H 3.951738609772E+00 -1.445600978670E+00 -2.719058924049E+00
H -2.390087979453E+00 -1.640640909528E-02 -3.079411380722E+00
H -8.731914568678E+00 1.416546671084E+00 -2.734307801002E+00
H 5.537195257079E+00 2.524985980156E+00 -1.762807256054E+00
H -8.046313321464E-01 3.054981430554E+00 -3.874688128737E-01
H -7.146457921372E+00 2.885117451730E+00 1.076634065830E+00
H 7.122651904385E+00 2.054307834148E+00 2.294093054899E+00
H -2.614797894719E+00 -7.437237547704E-01 2.988185724214E+00
H -8.956624483944E+00 -2.047213828495E+00 2.300281392835E+00
H 5.312485341813E+00 -2.881711885713E+00 1.085410315753E+00
H -1.029341247413E+00 -3.056044478307E+00 -3.781151840550E-01
H -7.371167836638E+00 -2.530274110249E+00 -1.755019051978E+00
H 6.897941989119E+00 -1.424848436642E+00 -2.729869205366E+00
H 5.561153998937E-01 6.992842514869E-03 -3.079339222294E+00

H -5.785711189331E+00 1.437232145724E+00 -2.723369733455E+00
H 8.483398636425E+00 2.538218884874E+00 -1.743509058845E+00
H 2.141572047200E+00 3.057730266352E+00 -3.642314704156E-01
H -4.200254542025E+00 2.876752493453E+00 1.098487158421E+00
H -1.054208113125E+01 2.036745392930E+00 2.309555617469E+00
H 3.727028694506E+00 7.301444683297E-01 2.991532717717E+00
H 8.701952508546E-01 -2.926915209802E+00 2.035611828025E+00
H -5.471631338371E+00 -3.537650694865E+00 4.422394384129E-01
H 8.797478487386E+00 -3.337953039047E+00 -1.252444676976E+00
H 2.455651898161E+00 -2.373570568677E+00 -2.660208810465E+00
H -3.886174691064E+00 -8.654316856506E-01 -3.458551164467E+00
H 1.038293513469E+01 8.409671669765E-01 -3.464581126750E+00
H 4.041108545467E+00 2.354710576402E+00 -2.676917305624E+00
H -2.300718043758E+00 3.329018170113E+00 -1.276003990129E+00
H -8.642544632983E+00 3.540687820069E+00 4.172264619889E-01
H 5.626565192773E+00 2.941228560361E+00 2.014875359789E+00
H -7.152613964516E-01 1.667969283121E+00 3.150940594542E+00
H -7.057087985677E+00 1.259834432663E-02 3.565163312036E+00
H 7.212021840080E+00 -1.645658723326E+00 3.162650079618E+00
H -2.243148050560E+00 -2.044361524619E+00 1.854021165299E+00
H -8.584974639785E+00 -2.671798827562E+00 6.915920399777E-01
H 5.684135185971E+00 -2.687159217777E+00 -6.292724871154E-01
H -6.576914032538E-01 -2.086923814978E+00 -1.805978270966E+00
H -6.999517992479E+00 -1.008599316326E+00 -2.568956197336E+00
H 7.269591833278E+00 3.007831307569E-01 -2.743417218174E+00
H 9.277652440524E-01 1.541259787413E+00 -2.289394416090E+00
H -5.414061345173E+00 2.428652400967E+00 -1.310898943474E+00
H 8.855048480584E+00 2.759670017893E+00 -3.209232095262E-02
H 2.513221891359E+00 2.458480491349E+00 1.254066265545E+00
H -3.828604697866E+00 1.594082712139E+00 2.252933383742E+00
H -1.017043128709E+01 3.644997943570E-01 2.735680614515E+00
H 4.098678538665E+00 -9.485856336134E-01 2.591716385028E+00

PBE0/POB-TZVP optimized geometry, *all*-[50.6]-$(SiMe_2)_\infty$

Energy (a.u): -1.070448671461E+04
Unit cell length (Å): 42.57772338

Si	-1.558331268253E+00	-1.161712217332E-03	1.526953862954E+00
Si	-8.899318058586E+00	-3.293844961324E-01	1.491004796395E+00
Si	-1.624030484892E+01	-6.422056270930E-01	1.385338002690E+00
Si	1.899643174468E+01	-9.249979366909E-01	1.214894343671E+00
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Si	-1.036751541665E+01	-1.524777347400E+00	8.150760713434E-02
Si	-1.770850220699E+01	-1.506650626538E+00	-2.481800530203E-01
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H 1.478821052440E+01 9.072428542140E-01 3.212467599349E+00
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H 1.202619658332E-01 -1.776848455619E+00 2.055173613025E+00
H -7.220724824500E+00 -2.177108302442E+00 1.625154901340E+00
H -1.456171161483E+01 -2.475568984724E+00 1.119145752699E+00
H 2.067502497877E+01 -2.658274812678E+00 5.608065925027E-01
H 1.333403818843E+01 -2.716682664851E+00 -2.375526066735E-02
H 5.993051398100E+00 -2.648061454992E+00 -6.072063442506E-01
H -1.347935392233E+00 -2.455619834606E+00 -1.162265134038E+00
H -8.688922182567E+00 -2.148356159979E+00 -1.662977697923E+00
H -1.602990897290E+01 -1.740637739039E+00 -2.085931272920E+00
H 1.920682762070E+01 -1.251529032000E+00 -2.411349019941E+00
H 1.186584083037E+01 -7.039002184004E-01 -2.624014766812E+00
H 4.524854040033E+00 -1.233578129169E-01 -2.713984499569E+00
H -2.816132750300E+00 4.629526667963E-01 -2.677051333504E+00
H -1.015711954063E+01 1.027615994345E+00 -2.514942222413E+00
H -1.749810633097E+01 1.544229140111E+00 -2.235237208160E+00
H 1.773863026263E+01 1.988635847573E+00 -1.851014986340E+00
H 1.039764347230E+01 2.340056153013E+00 -1.380241361015E+00
H 3.056656681966E+00 2.582058033523E+00 -8.449291836771E-01
H -4.284330108367E+00 2.703325750137E+00 -2.701090567815E-01
H -1.162531689870E+01 2.698188959206E+00 3.173410694045E-01
H -1.896630368903E+01 2.566887851363E+00 8.899526798845E-01
H 1.627043290457E+01 2.315561920482E+00 1.420951092164E+00
H 8.929446114233E+00 1.955962887762E+00 1.885507410648E+00
H 1.588459323900E+00 1.504905204306E+00 2.261899498201E+00
H -5.752527466434E+00 9.834798260787E-01 2.532527679139E+00
H -1.309351425677E+01 4.160680242434E-01 2.684737680503E+00
H -2.043450104710E+01 -1.707986559790E-01 2.711412331798E+00
H 1.480223554650E+01 -7.496789808770E-01 2.611304355977E+00
H 7.461248756167E+00 -1.293505149838E+00 2.389094690726E+00

PBE0/POB-TZVP optimized geometry, *all*-[35.9]-$(SiMe_2)_\infty$

Energy (a.u): -8.489747943006E+03
Unit cell length (Å): 28.98029187

Si	-1.561323179546E-03	-6.594734214627E-02	1.923342849404E+00
Si	-7.561637462192E+00	-5.824135264044E-01	1.834227699210E+00
Si	1.385857826501E+01	-1.055684763774E+00	1.609076271600E+00
Si	6.298502125997E+00	-1.450660691650E+00	1.264587017959E+00
Si	-1.261574013015E+00	-1.738047752358E+00	8.263091302963E-01
Si	-8.821650152027E+00	-1.896531762313E+00	3.267476745526E-01
Si	1.259856557517E+01	-1.914358687513E+00	-1.970471614414E-01
Si	5.038489436162E+00	-1.790206386468E+00	-7.062279109022E-01
Si	-2.521586702850E+00	-1.533282667388E+00	-1.163030966989E+00
Si	-1.008166284186E+01	-1.162642387170E+00	-1.533577336767E+00
Si	1.133855288534E+01	-7.057742398296E-01	-1.790385291126E+00
Si	3.778476746326E+00	-1.965620458238E-01	-1.914408558911E+00
Si	-3.781599392686E+00	3.272282559093E-01	-1.896448901717E+00
Si	-1.134167553170E+01	8.267495348712E-01	-1.737838305159E+00
Si	1.007854019550E+01	1.264954582959E+00	-1.450340191589E+00
Si	2.518464056491E+00	1.609343736411E+00	-1.055276980874E+00
Si	-5.041612082521E+00	1.834375227191E+00	-5.819487040581E-01
Si	-1.260168822153E+01	1.923359499079E+00	-6.545995410054E-02
Si	8.818527505668E+00	1.869696995704E+00	4.558836611933E-01
Si	1.258451366656E+00	1.677367619453E+00	9.434164708655E-01
Si	-6.301624772356E+00	1.360635560313E+00	1.360980396737E+00
Si	-1.386170091137E+01	9.429913861576E-01	1.677606632653E+00
Si	7.558514815832E+00	4.554098547898E-01	1.869812459165E+00
C	1.176898103821E+00	-1.065022714886E+00	3.001511517496E+00
C	-6.383178035191E+00	-1.835326899593E+00	2.602867638685E+00
C	-1.394325417420E+01	-2.469513284219E+00	2.011180974441E+00
C	7.476961552998E+00	-2.920547165826E+00	1.270334217862E+00
C	-8.311458601433E-02	-3.154977424758E+00	4.352725837374E-01
C	-7.643190725026E+00	-3.155417441157E+00	-4.320712266837E-01
C	1.377702500217E+01	-2.921834581020E+00	-1.267370290816E+00
C	6.216948863162E+00	-2.471552616512E+00	-2.008674298312E+00
C	-1.343127275850E+00	-1.837966901038E+00	-2.601004122175E+00
C	-8.903203414862E+00	-1.068067588654E+00	-3.000429369099E+00
C	1.251701231234E+01	-2.189545893032E-01	-3.177326495768E+00
C	4.956936173327E+00	6.463972702857E-01	-3.118575851547E+00
C	-2.603139965685E+00	1.463808801408E+00	-2.828534702952E+00
C	-1.016321610470E+01	2.172656330210E+00	-2.328714075125E+00
C	1.125699962250E+01	2.720367878241E+00	-1.656183377503E+00
C	3.696923483492E+00	3.066322185598E+00	-8.608211353071E-01
C	-3.863152655520E+00	3.184861403940E+00	-1.615727499993E-03

C -1.142322879453E+01 3.067194021724E+00 8.577095114244E-01
C 9.996986932668E+00 2.722046890394E+00 1.653422359646E+00
C 2.436910793656E+00 2.175017993741E+00 2.326508435357E+00
C -5.123165345356E+00 1.466677962537E+00 2.827048023486E+00
C -1.268324148437E+01 6.495611364562E-01 3.117918392596E+00
C 8.736974242833E+00 -2.157306675706E-01 3.177547018056E+00
C -1.177058961867E+00 8.560069100065E-01 3.071190675438E+00
C -8.737135100879E+00 -4.333476106323E-03 3.188250494529E+00
C 1.268308062632E+01 -8.643524681207E-01 3.068852359715E+00
C 5.123004487310E+00 -1.660266391724E+00 2.721851484447E+00
C -2.437071651702E+00 -2.333045952266E+00 2.172983336220E+00
C -9.997147790714E+00 -2.832794167504E+00 1.462954954683E+00
C 1.142306793649E+01 -3.122446998509E+00 6.444258967298E-01
C 3.862991797475E+00 -3.180522219880E+00 -2.218972819310E-01
C -3.697084341537E+00 -3.002712658122E+00 -1.071763354304E+00
C -1.125716048055E+01 -2.602205635009E+00 -1.842141641679E+00
C 1.016305524665E+01 -2.008704924245E+00 -2.475896710727E+00
C 2.602979107639E+00 -1.266227758463E+00 -2.926025847216E+00
C -4.957097031373E+00 -4.298402724434E-01 -3.159145032293E+00
C -1.251717317038E+01 4.384265001954E-01 -3.157964882452E+00
C 8.903042556816E+00 1.274177184983E+00 -2.922572924008E+00
C 1.342966417804E+00 2.015427976932E+00 -2.470427101672E+00
C -6.217109721208E+00 2.607203695802E+00 -1.835061002657E+00
C -1.377718586022E+01 3.005615043718E+00 -1.063596823920E+00
C 7.643029866981E+00 3.181113673615E+00 -2.132505343844E-01
C 8.295372796885E-02 3.120683654967E+00 6.529115717299E-01
C -7.477122411043E+00 2.828806805808E+00 1.470650213441E+00
C 1.394309331616E+01 2.327130296792E+00 2.179317456598E+00
C 6.383017177146E+00 1.652861179575E+00 2.726354693713E+00
H 1.922471018742E+00 -1.588833901710E+00 2.403969640893E+00
H -5.637605120270E+00 -2.178498877753E+00 1.886161668889E+00
H -1.319768125928E+01 -2.606594558003E+00 1.228465714519E+00
H 8.222534467919E+00 -2.841371044262E+00 4.796600779595E-01
H 6.624583289066E-01 -2.865416038576E+00 -3.047197522830E-01
H -6.897617810105E+00 -2.676946233714E+00 -1.066499912499E+00
H -1.445769394912E+01 -2.289939572913E+00 -1.749182653117E+00
H 6.962521778083E+00 -1.733098569764E+00 -2.302136518332E+00
H -5.975543609288E-01 -1.047721574095E+00 -2.684351449556E+00
H -8.157630499941E+00 -2.846398622828E-01 -2.867480313857E+00
H 1.326258522726E+01 4.995522859745E-01 -2.837941281129E+00
H 5.702509088248E+00 1.246694926481E+00 -2.597925126297E+00
H -1.857567050764E+00 1.901375907540E+00 -2.165232749564E+00
H -9.417643189776E+00 2.415040535752E+00 -1.571954965077E+00
H 1.200257253742E+01 2.749592655504E+00 -8.620924720454E-01
H 4.442496398413E+00 2.880220066546E+00 -8.829252417298E-02

H -3.117579740599E+00 2.797234731382E+00 6.920556763060E-01
H -1.067765587961E+01 2.506791292689E+00 1.421077273217E+00
H 1.074255984759E+01 2.030430611625E+00 2.044704069770E+00
H 3.182483708577E+00 1.403482180698E+00 2.516684519367E+00
H -4.377592430435E+00 6.724438969327E-01 2.802013991228E+00
H -1.193766856945E+01 -1.084664744420E-01 2.879530903720E+00
H 9.482547157754E+00 -8.813323836085E-01 2.743486182061E+00
H 6.344730023933E-01 -1.808480802134E+00 3.588826237991E+00
H -6.925603136619E+00 -2.709671159465E+00 2.967820544734E+00
H -1.448567927563E+01 -3.409897602819E+00 2.126705178549E+00
H 6.934536451570E+00 -3.857227540216E+00 1.127861818301E+00
H -6.255396874420E-01 -4.018484556597E+00 4.537010661291E-02
H -8.185615826454E+00 -3.881708956758E+00 -1.040486498328E+00
H 1.323459990075E+01 -3.457044761234E+00 -2.049174979596E+00
H 5.674523761735E+00 -2.775987370696E+00 -2.905885526980E+00
H -1.885552377277E+00 -1.889047696172E+00 -3.547079838370E+00
H -9.445628516289E+00 -8.620059958399E-01 -3.925203464958E+00
H 1.197458721091E+01 2.289667457883E-01 -4.012212707161E+00
H 4.414511071899E+00 1.302958071334E+00 -3.801654487526E+00
H -3.145565067113E+00 2.280314957366E+00 -3.309144945963E+00
H -1.070564120612E+01 3.088551314757E+00 -2.571211262089E+00
H 1.071457452108E+01 3.667723950314E+00 -1.642582601414E+00
H 3.154498382064E+00 3.974878279198E+00 -5.921311035084E-01
H -4.405577756948E+00 3.987234069971E+00 5.022360495252E-01
H -1.196565389596E+01 3.703874950157E+00 1.559354652342E+00
H 9.454561831241E+00 3.145816369389E+00 2.500823054168E+00
H 1.894485692229E+00 2.354446979657E+00 3.256816850571E+00
H -5.665590446783E+00 1.388459028322E+00 3.771267440112E+00
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H 8.194549141405E+00 -7.731636969576E-01 3.943665106964E+00
H 1.704813583543E+00 -4.153779141907E-01 3.701663475031E+00
H -5.855262555469E+00 -1.398671427830E+00 3.452328131993E+00
H -1.341533869448E+01 -2.278231880163E+00 2.946949404755E+00
H 8.004877032719E+00 -2.988826296162E+00 2.223008921563E+00
H 4.448008937074E-01 -3.477753138745E+00 1.334198036247E+00
H -7.115275245305E+00 -3.708750940689E+00 3.464357861336E-01
H 1.430494048190E+01 -3.664687651769E+00 -6.670200213996E-01
H 6.744864342884E+00 -3.348831244548E+00 -1.631006005359E+00
H -8.152117961280E-01 -2.784607343802E+00 -2.474027735257E+00
H -8.375287935140E+00 -2.013861855097E+00 -3.133562145955E+00
H 1.304492779206E+01 -1.093757445405E+00 -3.560694587380E+00
H 5.484851653049E+00 -9.253404959433E-02 -3.723746600353E+00
H -2.075224485963E+00 9.155521733596E-01 -3.610625362985E+00
H -9.635300624975E+00 1.855736079988E+00 -3.229720559957E+00
H 1.178491510223E+01 2.658288530991E+00 -2.609282157985E+00

H 4.224838963213E+00 3.263687882512E+00 -1.795325235026E+00
H -3.335237175799E+00 3.627034434165E+00 -8.482172524528E-01
H -1.089531331481E+01 3.721380434415E+00 1.617991233996E-01
H 1.052490241239E+01 3.539728672026E+00 1.159815598451E+00
H 2.964826273378E+00 3.095551427215E+00 2.071813856369E+00
H -4.595249865634E+00 2.421791294253E+00 2.830155158478E+00
H -1.215532600465E+01 1.568417979954E+00 3.378596799580E+00
H 9.264889722555E+00 5.987222791166E-01 3.676463372110E+00
H -1.704088695762E+00 1.594085735399E-01 3.725352026925E+00
H -9.264164834774E+00 -8.515906770748E-01 3.630213786618E+00
H 1.215605089243E+01 -1.799431342939E+00 3.265839196881E+00
H 4.595974753415E+00 -2.613816417948E+00 2.659252254131E+00
H -2.964101385597E+00 -3.234346686652E+00 1.855440736962E+00
H -1.052417752461E+01 -3.615000257759E+00 9.140196684088E-01
H 1.089603820259E+01 -3.727545797274E+00 -9.519005758842E-02
H 3.335962063580E+00 -3.563636317392E+00 -1.097339972480E+00
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H -5.484126765268E+00 3.493448687267E-01 -3.712360028409E+00
H -1.304420290428E+01 1.337972962380E+00 -3.480443530611E+00
H 8.376012822921E+00 2.227369722233E+00 -2.990398458118E+00
H 8.159366839091E-01 2.951572659327E+00 -2.278569212148E+00
H -6.744139455103E+00 3.456870954824E+00 -1.397748911475E+00
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H 7.116000133086E+00 3.679865523397E+00 6.018708728228E-01
H -4.440760059262E-01 3.381023309453E+00 1.572367704697E+00
H -8.004152144938E+00 2.831426063799E+00 2.426249217017E+00
H 1.341606358226E+01 2.071834899906E+00 3.100186924262E+00
H 5.855987443251E+00 1.158585219501E+00 3.544197949747E+00
H -1.923489682947E+00 1.421087584371E+00 2.513696586888E+00
H -9.483565821959E+00 6.902025790155E-01 2.803886740456E+00
H 1.193664990524E+01 -9.187159415901E-02 2.886125441413E+00
H 4.376573766229E+00 -8.671320714794E-01 2.754313421526E+00
H -3.183502372783E+00 -1.578081329923E+00 2.418226575310E+00
H -1.074357851179E+01 -2.171991515369E+00 1.902790926653E+00
H 1.067663721541E+01 -2.604815026319E+00 1.246233979656E+00
H 3.116561076394E+00 -2.844451323003E+00 4.972495595286E-01
H -4.443515062618E+00 -2.873127677559E+00 -2.886135856634E-01
H -1.200359120163E+01 -2.688717295955E+00 -1.053071581526E+00
H 9.416624525571E+00 -2.304897052573E+00 -1.739428075669E+00
H 1.856548386559E+00 -1.750133139004E+00 -2.296779146793E+00
H -5.703527752453E+00 -1.065569856842E+00 -2.683788615666E+00
H -1.326360389147E+01 -3.019781330554E-01 -2.871753760430E+00

H 8.156611835735E+00 4.840099274020E-01 -2.846734066182E+00
H 5.965356967232E-01 1.234101185742E+00 -2.610585129188E+00
H -6.963540442289E+00 1.892664804773E+00 -2.180821035794E+00
H 1.445667528491E+01 2.410858133599E+00 -1.589315422767E+00
H 6.896599145900E+00 2.750249143598E+00 -8.799375554685E-01
H -6.634769931121E-01 2.885666756169E+00 -1.052987451270E-01
H -8.223553132124E+00 2.807067666482E+00 6.771495914308E-01
H 1.319666259508E+01 2.520281209453E+00 1.409376840545E+00
H 5.636586456065E+00 2.046577024637E+00 2.037077056867E+00
H -6.324570447435E-01 1.555988254358E+00 3.707872563621E+00
H -8.192533183755E+00 4.979159435047E-01 3.990175197778E+00
H 1.322768254345E+01 -5.970845150645E-01 3.976544791352E+00
H 5.667606404433E+00 -1.647801946631E+00 3.667992249233E+00
H -1.892469734579E+00 -2.576309446009E+00 3.087401501937E+00
H -9.452545873591E+00 -3.313743859607E+00 2.277832309164E+00
H 1.196766985361E+01 -3.805413050508E+00 1.299326714410E+00
H 4.407593714598E+00 -4.014852164059E+00 2.244560012724E-01
H -3.152482424414E+00 -3.926528059328E+00 -8.670615866617E-01
H -1.071255856343E+01 -3.546991331108E+00 -1.894273183256E+00
H 1.070765716377E+01 -2.904390482265E+00 -2.780995203571E+00
H 3.147581024763E+00 -2.046384278054E+00 -3.461463531844E+00
H -4.412495114249E+00 -1.036607113526E+00 -3.885210945102E+00
H -1.197257125326E+01 5.005045845084E-02 -4.020810036220E+00
H 9.447644473939E+00 1.132996016890E+00 -3.858204040932E+00
H 1.887568334927E+00 2.131912443868E+00 -3.409452702038E+00
H -5.672507804085E+00 2.972714677735E+00 -2.707837853442E+00
H -1.323258394310E+01 3.593044263219E+00 -1.805395058790E+00
H 8.187631784104E+00 3.946894192784E+00 -7.690543717608E-01
H 6.275556450919E-01 4.008021035910E+00 3.243235598326E-01
H -6.932520493920E+00 3.771891294278E+00 1.393647896675E+00
H 1.448769523328E+01 3.256017630604E+00 2.359611744536E+00
H 6.927619094269E+00 2.498660034558E+00 3.150573983810E+00

PbE0/POB-TZVP optimized geometry, *all*-[180]-$(GeMe_2)_\infty$

Energy (a.u): -4.3130233529175E+03
Unit cell length (Å): 4.0062192

Coordinates (Å):

Ge	-4.451557800657E-01	1.085369734678E-03	-6.775167489120E-01
Ge	1.557953819934E+00	-1.085369734678E-03	6.775167489120E-01
C	-4.874255400016E-01	1.586191067213E+00	-1.835963700597E+00
C	1.515684059998E+00	-1.586191067213E+00	1.835963700597E+00
C	-4.028650681450E-01	-1.580311659532E+00	-1.841018847741E+00
C	1.600244531855E+00	1.580311659532E+00	1.841018847741E+00
H	4.976833940366E-01	1.817131009524E+00	-2.241252811823E+00
H	-1.505426205963E+00	-1.817131009524E+00	2.241252811823E+00
H	-1.157310228735E+00	1.428457585282E+00	-2.682731864279E+00
H	8.457993712645E-01	-1.428457585282E+00	2.682731864279E+00
H	1.947767573467E+00	2.467841521103E+00	1.312173416351E+00
H	-5.534202653255E-02	-2.467841521103E+00	-1.312173416351E+00
H	2.671769009766E-01	-1.419943536243E+00	-2.687167102594E+00
H	-1.735932699023E+00	1.419943536243E+00	2.687167102594E+00
H	1.167980043793E+00	-2.471990300306E+00	1.304343520107E+00
H	-8.351295562069E-01	2.471990300306E+00	-1.304343520107E+00
H	-1.387931419709E+00	-1.809849873168E+00	-2.247207925821E+00
H	6.151781802905E-01	1.809849873168E+00	2.247207925821E+00

PbE0/POB-TZVP optimized geometry, *all*-[163.2]-$(GeMe_2)_\infty$

Energy (a.u): -2.803465947577E+04
Unit cell length (Å): 25.79322302

Ge	-2.144980234840E-05	-3.078745723133E-01	6.187647411170E-01
Ge	-3.968209606725E+00	-5.601637084409E-01	4.048125206467E-01
Ge	-7.936397763648E+00	-6.841260896693E-01	9.812263021604E-02
Ge	-1.190458592057E+01	-6.513634283675E-01	-2.310459722913E-01
Ge	9.920448942505E+00	-4.693812554070E-01	-5.072847269525E-01
Ge	5.952260785582E+00	-1.798694934901E-01	-6.673106641125E-01
Ge	1.984072628659E+00	1.508482017230E-01	-6.744637700897E-01
Ge	-1.984115528264E+00	4.470083918393E-01	-5.271053545089E-01
Ge	-5.952303685187E+00	6.407643464203E-01	-2.589934545182E-01
Ge	-9.920491842110E+00	6.877289112839E-01	6.845072469306E-02
Ge	1.190454302097E+01	5.771430706042E-01	3.802136677978E-01
Ge	7.936354864044E+00	3.343407077770E-01	6.048742416816E-01
Ge	3.968166707121E+00	1.494491804052E-02	6.909654163209E-01
C	-1.049540228730E-01	-2.239118323094E+00	9.495197510177E-01
C	-4.073142179796E+00	-2.423904641945E+00	-1.998121846742E-01
C	-8.041330336719E+00	-2.053403618544E+00	-1.303369556855E+00
C	-1.200951849364E+01	-1.212492572331E+00	-2.108340670866E+00
C	9.815516369435E+00	-9.381408991654E-02	-2.430316345442E+00
C	5.847328212512E+00	1.046356069916E+00	-2.195535833763E+00
C	1.879140055589E+00	1.946818664088E+00	-1.457784521645E+00
C	-2.089048101334E+00	2.401288564026E+00	-3.860723438254E-01
C	-6.057236258258E+00	2.305652192610E+00	7.740843552883E-01
C	-1.002542441518E+01	1.681818689988E+00	1.756907657333E+00
C	1.179961044790E+01	6.727007936020E-01	2.337244588116E+00
C	7.831422290973E+00	-4.905247476746E-01	2.382146950611E+00
C	3.863234134050E+00	-1.541376980723E+00	1.881328154705E+00
C	1.049649382629E-01	5.930839422030E-01	2.358696383595E+00
C	-3.863223218660E+00	-5.709911149306E-01	2.364141776449E+00
C	-7.831411375583E+00	-1.604258988823E+00	1.827990779316E+00
C	-1.179959953251E+01	-2.270010461792E+00	8.730691243188E-01
C	1.002543533057E+01	-2.415729894556E+00	-2.818621454366E-01
C	6.057247173648E+00	-2.008034721179E+00	-1.372222194480E+00
C	2.089059016724E+00	-1.140322992621E+00	-2.148222675837E+00
C	-1.879129140199E+00	-1.137700883609E-02	-2.432091231051E+00
C	-5.847317297122E+00	1.120175310566E+00	-2.158796995107E+00
C	-9.815505454045E+00	1.995108965893E+00	-1.390948383908E+00
C	1.200952940903E+01	2.412987200804E+00	-3.044502607012E-01
C	8.041341252109E+00	2.278079147658E+00	8.517937482089E-01
C	4.073153095186E+00	1.621290615614E+00	1.812902074632E+00
H	-9.423169519554E-01	-2.483257582131E+00	1.604931430716E+00

H -4.910505108878E+00 -2.944664214742E+00 2.670688655181E-01
H -8.878693265802E+00 -2.731483762806E+00 -1.131975958241E+00
H -1.284688142272E+01 -1.892553298760E+00 -2.271698731757E+00
H 8.978153440352E+00 -6.200616817067E-01 -2.891002702764E+00
H 5.009965283429E+00 7.944785940718E-01 -2.848012794928E+00
H 1.041777126506E+00 2.027013398454E+00 -2.152577478048E+00
H -2.926411030417E+00 2.795183861409E+00 -9.640126023188E-01
H -6.894599187340E+00 2.923011387333E+00 4.453959429908E-01
H -1.086278734426E+01 2.381212230525E+00 1.752769645364E+00
H 1.096224751881E+01 1.293906048422E+00 2.658604945149E+00
H 6.994059361891E+00 -8.981841611658E-02 2.955385891662E+00
H 3.025871204968E+00 -1.452966563952E+00 2.575123546657E+00
H 8.017823400425E-01 -2.610626339737E+00 1.428442828914E+00
H -3.166405816881E+00 -2.975425305785E+00 5.160475653943E-02
H -7.134593973804E+00 -2.658590192040E+00 -1.337055343654E+00
H -1.110278213073E+01 -1.732704104784E+00 -2.419412177879E+00
H 1.072225273235E+01 -4.098763884694E-01 -2.947510839230E+00
H 6.754064575427E+00 1.006849068897E+00 -2.800370288670E+00
H 2.785876418504E+00 2.192917538426E+00 -2.011698653096E+00
H -1.182311738419E+00 2.876615027423E+00 -7.621710996942E-01
H -5.150499895342E+00 2.901314680606E+00 6.619606674898E-01
H -9.118688052265E+00 2.261358105095E+00 1.934445223243E+00
H 1.270634681081E+01 1.103351640026E+00 2.763771690943E+00
H 8.738158653889E+00 -3.074193889447E-01 2.959951371308E+00
H 4.769970496966E+00 -1.647764340713E+00 2.478041863787E+00
H -2.385691036005E-01 -2.798992515877E+00 2.373949047433E-02
H -4.206757260524E+00 -2.489417080257E+00 -1.279736405619E+00
H -8.174945417447E+00 -1.609546192279E+00 -2.290040113680E+00
H -1.214313357437E+01 -3.609476687837E-01 -2.775723229672E+00
H 9.681901288707E+00 9.703396157389E-01 -2.625521604838E+00
H 5.713713131784E+00 2.079333788156E+00 -1.873844621301E+00
H 1.745524974861E+00 2.711977648395E+00 -6.928924172989E-01
H -2.222663182062E+00 2.723340112260E+00 6.467930892471E-01
H -6.190851338985E+00 2.110818176213E+00 1.838306093748E+00
H -1.015903949591E+01 1.014733234112E+00 2.608685326162E+00
H 1.166599536717E+01 -3.138148630629E-01 2.781446188418E+00
H 7.697807210246E+00 -1.570471756989E+00 2.317011248968E+00
H 3.729619053323E+00 -2.467352497626E+00 1.321776955392E+00
H 2.379473029201E-01 1.669287919036E+00 2.246871993198E+00
H -3.730240854003E+00 4.339075666053E-01 2.765263122037E+00
H -7.698429010926E+00 -9.008757801817E-01 2.650165794651E+00
H -1.166661716785E+01 -2.029279342459E+00 1.927947421670E+00
H 1.015841769523E+01 -2.692799462846E+00 7.640595286702E-01
H 6.190229538305E+00 -2.739431678047E+00 -5.748651944329E-01
H 2.222041381382E+00 -2.158493109537E+00 -1.782095229368E+00

H -1.746146775541E+00 -1.083069782295E+00 -2.581068723831E+00
H -5.714334932465E+00 2.404717796656E-01 -2.788750478914E+00
H -9.682523089388E+00 1.508924154904E+00 -2.357563107364E+00
H 1.214251177369E+01 2.431700190761E+00 -1.386286439633E+00
H 8.174323616766E+00 2.797403018079E+00 -9.742825514448E-02
H 4.206135459843E+00 2.522254526316E+00 1.213749568460E+00
H 9.426995847606E-01 2.179917199157E-01 2.948468158968E+00
H -3.025488572162E+00 -1.177199393564E+00 2.712044701363E+00
H -6.993676729086E+00 -2.302708312768E+00 1.854324486358E+00
H -1.096186488601E+01 -2.900694508161E+00 5.718008785607E-01
H 1.086316997707E+01 -2.834166548893E+00 -8.417154195673E-01
H 6.894981820145E+00 -2.118365188682E+00 -2.062404858843E+00
H 2.926793663222E+00 -9.172718928129E-01 -2.810622199630E+00
H -1.041394493701E+00 4.939573393754E-01 -2.914959866152E+00
H -5.009582650624E+00 1.792026897944E+00 -2.351515356413E+00
H -8.977770807547E+00 2.679564690459E+00 -1.249367017351E+00
H 1.284726405553E+01 2.953246504645E+00 1.389962488803E-01
H 8.879075898607E+00 2.550375135095E+00 1.495517149580E+00
H 4.910887741684E+00 1.563243557448E+00 2.509433094246E+00
H -8.015326377553E-01 4.346254493447E-01 2.944098743021E+00
H -4.769720794678E+00 -9.833491836423E-01 2.808850489596E+00
H -8.737908951601E+00 -2.176050369299E+00 2.030128439323E+00
H -1.270609710852E+01 -2.870244639599E+00 7.863284293010E-01
H 9.118937754552E+00 -2.906900453165E+00 -6.376099475893E-01
H 5.150749597629E+00 -2.277620404859E+00 -1.915479569520E+00
H 1.182561440706E+00 -1.126564970101E+00 -2.754535906104E+00
H -2.785626716217E+00 2.825729227279E-01 -2.962561262357E+00
H -6.753814873140E+00 1.626976764332E+00 -2.491899536137E+00
H -1.072200303006E+01 2.598659836424E+00 -1.450373656833E+00
H 1.110303183301E+01 2.975021257236E+00 -7.658465164572E-02
H 7.134843676091E+00 2.669841160909E+00 1.314748974288E+00
H 3.166655519168E+00 1.753032629691E+00 2.404889454656E+00

PbE0/POB-TZVP optimized geometry, *all*-[149.0]-$(GeMe_2)_\infty$

Energy (a.u): -1.5095576536249E+04
Unit cell length (Å): 13.9475030100

Ge	1.288272669889E-04	9.048301655697E-03	-7.030291476793E-01
Ge	-3.984872032733E+00	5.552918445548E-01	-4.312572568902E-01
Ge	5.977630117267E+00	6.833893026148E-01	1.652601443821E-01
Ge	1.992629257267E+00	2.968806772046E-01	6.373332862421E-01
Ge	-1.992371602733E+00	-3.131851534029E-01	6.294814643320E-01
Ge	-5.977372462733E+00	-6.874161756851E-01	1.476172606981E-01
Ge	3.985129687267E+00	-5.440087969419E-01	-4.454057510848E-01
C	-1.364292115035E-01	1.596024057672E+00	-1.848868471264E+00
C	-4.121430071504E+00	2.440608301256E+00	9.507121825309E-02
C	5.841072078496E+00	1.447364714658E+00	1.967420341326E+00
C	1.856071218496E+00	-6.357740229372E-01	2.358261819320E+00
C	-2.128929641504E+00	-2.240161953834E+00	9.732840475909E-01
C	-6.113930501504E+00	-2.157662242518E+00	-1.144596463350E+00
C	3.848571648496E+00	-4.503988542970E-01	-2.400572491876E+00
C	1.364164036151E-01	-1.547865887248E+00	-1.889471592563E+00
C	-3.848584456385E+00	5.121697809506E-01	-2.388236550154E+00
C	6.113917693615E+00	2.186531157734E+00	-1.088610674331E+00
C	2.128916833615E+00	2.214389975636E+00	1.030761242874E+00
C	-1.856084026385E+00	5.747679765610E-01	2.373948920497E+00
C	-5.841084886385E+00	-1.497666031995E+00	1.929504641253E+00
C	4.121417263615E+00	-2.442326971639E+00	3.210401242399E-02
H	-8.604830559840E-01	1.441856090419E+00	-2.649014207172E+00
H	-4.845483915984E+00	2.970065272796E+00	-5.243448584728E-01
H	5.117018234016E+00	2.261754726468E+00	1.995166863342E+00
H	1.132017374016E+00	-1.497032602797E-01	3.012277243074E+00
H	-2.852983485984E+00	-2.448431638646E+00	1.761081419513E+00
H	-6.837984345984E+00	-2.903441054209E+00	-8.162446324554E-01
H	3.124517804016E+00	-1.172100136548E+00	-2.778921827828E+00
H	8.203119251122E-01	1.827013626178E+00	-2.319051167753E+00
H	-3.164688934888E+00	2.952231576182E+00	-1.748798123855E-02
H	6.797813215112E+00	1.854358934772E+00	2.297244011838E+00
H	2.812812355112E+00	-6.398838065503E-01	2.882104408763E+00
H	-1.172188504888E+00	-2.652280990289E+00	1.296681401673E+00
H	-5.157189364888E+00	-2.667456491668E+00	-1.265169148357E+00
H	4.805312785112E+00	-6.739828486246E-01	-2.874321524927E+00
H	-4.445136186164E-01	2.480098413325E+00	-1.290444124021E+00
H	-4.429514478616E+00	2.555225910840E+00	1.134440267961E+00
H	5.532987671384E+00	7.062161803824E-01	2.705067999804E+00
H	1.547986811384E+00	-1.674588738087E+00	2.238724354464E+00
H	-2.437014048616E+00	-2.794394181393E+00	8.657560855756E-02

H -6.422014908616E+00 -1.809963810856E+00 -2.130766336413E+00
H 3.540487241384E+00 5.374062257887E-01 -2.743597770352E+00
H 4.487793053692E-01 -2.445067601912E+00 -1.354847669250E+00
H -3.536221554631E+00 -4.652121528792E-01 -2.756364532787E+00
H 6.426280595369E+00 1.864957535870E+00 -2.082282683545E+00
H 2.441279735369E+00 2.790776161908E+00 1.598004972316E-01
H -1.543721124631E+00 1.615083416571E+00 2.281550644257E+00
H -5.528721984631E+00 -7.768000831425E-01 2.685246621006E+00
H 4.433780165369E+00 -2.583737276415E+00 1.066897123088E+00
H 8.572000136599E-01 -1.371448149018E+00 -2.687974518343E+00
H -3.127800846340E+00 1.246459167822E+00 -2.748166039318E+00
H 6.834701303660E+00 2.925757308158E+00 -7.389324803153E-01
H 2.849700443660E+00 2.401900520879E+00 1.826732307840E+00
H -1.135300416340E+00 6.936365153624E-02 3.016830409644E+00
H -5.120301276340E+00 -2.315405462174E+00 1.935193680860E+00
H 4.842200873660E+00 -2.956627037203E+00 -6.036833603682E-01
H -8.214105889194E-01 -1.769378361063E+00 -2.362007468484E+00
H -4.806411448919E+00 7.435024369331E-01 -2.856043275591E+00
H 5.156090701081E+00 2.696510735233E+00 -1.199420243512E+00
H 1.171089841081E+00 2.618991451107E+00 1.360390695645E+00
H -2.813911018919E+00 5.693181866085E-01 2.895799694069E+00
H -6.798911878919E+00 -1.909063284381E+00 2.250612459310E+00
H 3.163590271081E+00 -2.949881164438E+00 -8.933186143720E-02

PbE0/POB-TZVP optimized geometry, *all*-[130.4]-$(GeMe_2)_\infty$

Energy (a.u): -2.8034625152808E+04
Unit cell length (Å): 25.93847948

Ge	-6.458840278979E-05	9.546123497894E-03	-7.398852050992E-01
Ge	9.976273673136E+00	3.522944720348E-01	-6.506995083541E-01
Ge	-5.985867545326E+00	6.143364026372E-01	-4.124463960242E-01
Ge	3.990470716213E+00	7.356412669516E-01	-7.970678488309E-02
Ge	-1.197167050225E+01	6.884195824457E-01	2.712926901039E-01
Ge	-1.995332240710E+00	4.834892679569E-01	5.601422792193E-01
Ge	7.981006020828E+00	1.677973888564E-01	7.206700226119E-01
Ge	-7.981135197634E+00	-1.863348498533E-01	7.161009488394E-01
Ge	1.995203063905E+00	-4.977800200400E-01	5.474817776397E-01
Ge	1.197154132544E+01	-6.951897865350E-01	2.534411290534E-01
Ge	-3.990599893018E+00	-7.333399508801E-01	-9.865982790228E-02
Ge	5.985738368520E+00	-6.034907701830E-01	-4.281590072654E-01
Ge	-9.976402849941E+00	-3.353891268891E-01	-6.595721179394E-01
C	2.232226510699E-01	1.570115229872E+00	-1.907199108913E+00
C	1.019956091261E+01	2.276587610873E+00	-9.590720130071E-01
C	-5.762580305853E+00	2.461521206078E+00	2.087669230080E-01
C	4.213757955685E+00	2.082549957517E+00	1.328779872876E+00
C	-1.174838326278E+01	1.226491611136E+00	2.144385367402E+00
C	-1.772045001238E+00	8.945881747053E-02	2.468738016901E+00
C	8.204293260301E+00	-1.068067913182E+00	2.227532538246E+00
C	-7.757847958161E+00	-1.980913156538E+00	1.476026199757E+00
C	2.218490303378E+00	-2.439955068323E+00	3.863800469466E-01
C	1.219482856492E+01	-2.340032678601E+00	-7.917811182343E-01
C	-3.767312653545E+00	-1.704037002663E+00	-1.788554771225E+00
C	6.209025607993E+00	-6.776669852862E-01	-2.375592080549E+00
C	-9.753115610469E+00	5.039483716469E-01	-2.418409873208E+00
C	-2.232383034446E-01	-1.520404456599E+00	-1.947074035034E+00
C	9.753099958094E+00	-4.414008657605E-01	-2.430615618574E+00
C	-6.209041260368E+00	7.387223439666E-01	-2.357332455992E+00
C	3.767297001171E+00	1.749613167260E+00	-1.744012836678E+00
C	-1.219484421729E+01	2.359688699059E+00	-7.311608941147E-01
C	-2.218505955752E+00	2.429187987235E+00	4.491911978467E-01
C	7.757832305786E+00	1.942189582424E+00	1.526638999722E+00
C	-8.204308912675E+00	1.010258950202E+00	2.254352204756E+00
C	1.772029348863E+00	-1.531098325718E-01	2.465620487569E+00
C	1.174836761040E+01	-1.281402997877E+00	2.112044830628E+00
C	-4.213773608060E+00	-2.116142178948E+00	1.274625155890E+00
C	5.762564653478E+00	-2.466098689100E+00	1.452042188354E-01
C	-1.019957656498E+01	-2.251101709291E+00	-1.017481254854E+00
H	-6.908265783486E-01	1.760995811680E+00	-2.471846872846E+00

H 9.285511683190E+00 2.708008872158E+00 -1.370336148494E+00
H -6.676629535272E+00 3.034649735069E+00 4.510207313748E-02
H 3.299708726267E+00 2.666088915169E+00 1.450207953352E+00
H -1.266243249219E+01 1.686759254659E+00 2.523088668354E+00
H -2.686094230656E+00 3.210133765591E-01 3.017960175951E+00
H 7.290244030882E+00 -1.118272797480E+00 2.821453377600E+00
H -8.671897187579E+00 -2.301376150265E+00 1.978585612640E+00
H 1.304441073959E+00 -2.957261961613E+00 6.824477283662E-01
H 1.128077933550E+01 -2.935674696425E+00 -7.700307060898E-01
H -4.681361882964E+00 -2.241559737002E+00 -2.046104385657E+00
H 5.294976378574E+00 -1.033930455555E+00 -2.853440208700E+00
H -1.066716483989E+01 4.105598330467E-01 -3.007087267613E+00
H 1.024264462976E+00 1.416842451164E+00 -2.629594726568E+00
H 1.100060272451E+01 2.476585288305E+00 -1.669950977474E+00
H -4.961538493947E+00 2.968972281983E+00 -3.277415845322E-01
H 5.014799767592E+00 2.781203505854E+00 1.089549455712E+00
H -1.094734145087E+01 1.956294523669E+00 2.257237846147E+00
H -9.710031893315E-01 6.832220420164E-01 2.907820248694E+00
H 9.005335072207E+00 -7.463683757439E-01 2.892256075299E+00
H -6.956806146255E+00 -2.004974793335E+00 2.214110890517E+00
H 3.019532115284E+00 -2.804265648339E+00 1.028739583646E+00
H -1.294260910318E+01 -2.961133038373E+00 -3.923035641823E-01
H -2.966270841639E+00 -2.439640534837E+00 -1.723474693227E+00
H 7.010067419899E+00 -1.359255785626E+00 -2.659818540175E+00
H -8.952073798562E+00 3.251808326418E-02 -2.986830013857E+00
H 4.497965864248E-01 2.477688401492E+00 -1.347790958884E+00
H 1.042613484796E+01 2.820233814457E+00 -4.197041258734E-02
H -5.536006370498E+00 2.516697648031E+00 1.273465049435E+00
H 4.440331891040E+00 1.636616379936E+00 2.297165015549E+00
H -1.152180932742E+01 3.816060225634E-01 2.794612160440E+00
H -1.545471065883E+00 -9.608256757276E-01 2.651847338102E+00
H 8.430867195656E+00 -2.083143790914E+00 1.901576248830E+00
H -7.531274022806E+00 -2.728238768206E+00 7.156769574286E-01
H 2.445064238733E+00 -2.748327122544E+00 -6.341753000773E-01
H 1.242140250027E+01 -2.138806854039E+00 -1.838745638976E+00
H -3.540738718191E+00 -1.039311710690E+00 -2.622081511273E+00
H 6.435599543348E+00 2.982772205134E-01 -2.804730108845E+00
H -9.526541675114E+00 1.567534435128E+00 -2.344848839142E+00
H -4.497464996316E-01 -2.442101468360E+00 -1.411223008881E+00
H 9.526591761907E+00 -1.506545427268E+00 -2.384477057583E+00
H -6.435549456555E+00 -2.258579846287E-01 -2.811476148457E+00
H 3.540788804984E+00 1.106570800405E+00 -2.594399935679E+00
H -1.242135241348E+01 2.185497550689E+00 -1.782977963546E+00
H -2.445014151939E+00 2.763753150212E+00 -5.630972271788E-01
H 7.531324109599E+00 2.708866209857E+00 7.857822978782E-01

H -8.430817108862E+00 2.033410666200E+00 1.954648568195E+00
H 1.545521152676E+00 8.921252441721E-01 2.675728407606E+00
H 1.152185941421E+01 -4.535353200209E-01 2.783831114859E+00
H -4.440281804247E+00 -1.695296408090E+00 2.254191662498E+00
H 5.536056457292E+00 -2.548685519603E+00 1.208144066214E+00
H -1.042608476117E+01 -2.818201493564E+00 -1.146747759251E-01
H 6.908486148902E-01 -1.696606703231E+00 -2.516408386176E+00
H 1.066718687643E+01 -3.328373411583E-01 -3.016621417380E+00
H -5.294954342033E+00 1.107181044649E+00 -2.825762836091E+00
H 4.681383919506E+00 2.293557596105E+00 -1.987556043188E+00
H -1.128075729896E+01 2.954507742659E+00 -6.940241134371E-01
H -1.304419037417E+00 2.938615771048E+00 7.585003768049E-01
H 8.671919224121E+00 2.249522340449E+00 2.037261571641E+00
H -7.290221994341E+00 1.045090451336E+00 2.849310692078E+00
H 2.686116267198E+00 -3.987590654729E-01 3.008617070876E+00
H 1.266245452874E+01 -1.751257685950E+00 2.478685536503E+00
H -3.299686689725E+00 -2.702564275518E+00 1.380917017115E+00
H 6.676651571813E+00 -3.034745958996E+00 -3.320294903909E-02
H -9.285489646648E+00 -2.671703915921E+00 -1.439716519708E+00
H -1.024256348128E+00 -1.348650987124E+00 -2.665323224848E+00
H 8.952081913411E+00 4.446632052119E-02 -2.986775874471E+00
H -7.010059305051E+00 1.427396930012E+00 -2.623994165805E+00
H 2.966278956488E+00 2.483328104835E+00 -1.660087016310E+00
H 1.294261721803E+01 2.970358738188E+00 -3.158739375956E-01
H -3.019524000435E+00 2.776915981326E+00 1.100702053528E+00
H 6.956814261103E+00 1.947315238607E+00 2.265120469086E+00
H -9.005326957358E+00 6.716080424161E-01 2.910627082837E+00
H 9.710113041801E-01 -7.579564625383E-01 2.889344108770E+00
H 1.094734956572E+01 -2.013882276291E+00 2.206147219754E+00
H -5.014791652743E+00 -2.808451930457E+00 1.017548589649E+00
H 4.961546608795E+00 -2.959639092871E+00 -4.041581595553E-01
H -1.100059460967E+01 -2.432808606625E+00 -1.733277145039E+00

PbE0/POB-TZVP optimized geometry, *all*-[121.5]-$(GeMe_2)_\infty$

Energy (a.u): -2.3721598486395E+04
Unit cell length (Å): 21.8213128300

Ge	-6.589727538064E-06	-7.552760701796E-01	1.621908812596E-01
Ge	5.951260545727E+00	-7.230656729295E-01	-2.718894201339E-01
Ge	-9.918785148818E+00	-4.612870334621E-01	-6.196467517137E-01
Ge	-3.967518013364E+00	-5.305302016902E-02	-7.706706178392E-01
Ge	1.983749122091E+00	3.720249521730E-01	-6.770120080991E-01
Ge	7.935016257545E+00	6.789876308029E-01	-3.684068693258E-01
Ge	-7.935029437000E+00	7.703765341501E-01	5.716484741992E-02
Ge	-1.983762301546E+00	6.171763311252E-01	4.645871290173E-01
Ge	3.967504833909E+00	2.680270037276E-01	7.245062797675E-01
Ge	9.918771969363E+00	-1.662190035652E-01	7.543998058082E-01
Ge	-5.951273725182E+00	-5.476916516734E-01	5.447767238392E-01
C	-2.946637322109E-01	-2.251291294655E+00	-1.071894047683E+00
C	5.656603403244E+00	-1.314397080895E+00	-2.118874620307E+00
C	-1.021344229130E+01	3.980891896238E-02	-2.493127472236E+00
C	-4.262175155847E+00	1.381375868326E+00	-2.075829967327E+00
C	1.689091979607E+00	2.284365739832E+00	-9.994711149057E-01
C	7.640359115062E+00	2.462085629498E+00	3.942127545730E-01
C	-8.229686579484E+00	1.858110728064E+00	1.662736859849E+00
C	-2.278419444029E+00	6.641987992531E-01	2.403353760460E+00
C	3.672847691425E+00	-7.405915553163E-01	2.380922823412E+00
C	9.624114826880E+00	-1.910249323843E+00	1.602565712726E+00
C	-6.245930867665E+00	-2.473416429226E+00	3.154053114389E-01
C	2.946565907913E-01	-1.612752959830E+00	1.901656254096E+00
C	6.245923726246E+00	-2.384847116775E+00	7.278549634323E-01
C	-9.624121968300E+00	-2.399769164668E+00	-6.770351353437E-01
C	-3.672854832845E+00	-1.652781458738E+00	-1.866971362350E+00
C	2.278412302609E+00	-3.810473176545E-01	-2.464157373199E+00
C	8.229679438064E+00	1.011666654433E+00	-2.278990828962E+00
C	-7.640366256481E+00	2.083183611833E+00	-1.370260799109E+00
C	-1.689099121027E+00	2.493304491548E+00	-2.648264733886E-02
C	4.262168014428E+00	2.111818812044E+00	1.325703557844E+00
C	1.021343514988E+01	1.059845581115E+00	2.256988250384E+00
C	-5.656610544663E+00	-3.286211333069E-01	2.471695120545E+00
H	-1.157081170661E+00	-2.848333112281E+00	-7.760041903893E-01
H	4.794185964794E+00	-1.976630753545E+00	-2.192741408866E+00
H	1.074545310025E+01	-4.773620967646E-01	-2.913298723199E+00
H	-5.124592594297E+00	1.173465652859E+00	-2.708904277301E+00
H	8.266745411572E-01	2.451726349013E+00	-1.644451863563E+00
H	6.777941676612E+00	2.951581252425E+00	-5.789760228509E-02
H	-9.092104017934E+00	2.514329963069E+00	1.547038738633E+00

H -3.140836882479E+00 1.278796675845E+00 2.660801210888E+00
H 2.810430252975E+00 -3.627455204141E-01 2.929778099010E+00
H 8.761697388430E+00 -1.889118576979E+00 2.268571141518E+00
H -7.108348306116E+00 -2.815709833227E+00 8.871088755526E-01
H 5.717028118695E-01 -2.914937256210E+00 -1.073633864228E+00
H 6.522969947324E+00 -1.871750974764E+00 -2.479132342278E+00
H -9.347075747221E+00 -2.342969839903E-01 -3.097523818367E+00
H -3.395808611767E+00 1.477544643737E+00 -2.732473368182E+00
H 2.555458523688E+00 2.720276286909E+00 -1.499881930333E+00
H 8.506725659142E+00 3.099339429541E+00 2.089114227370E-01
H -7.363320035403E+00 2.494384202180E+00 1.851376875186E+00
H -1.412052899949E+00 1.097479615104E+00 2.906043250967E+00
H 4.539214235506E+00 -6.478669953481E-01 3.038061427687E+00
H 1.049048137096E+01 -2.187520412386E+00 2.205516567032E+00
H -5.379564323585E+00 -3.032651554772E+00 6.727357797802E-01
H -4.537513530331E-01 -1.927835479838E+00 -2.099708403611E+00
H 5.497515782421E+00 -4.866103403844E-01 -2.808653662193E+00
H -1.037252991212E+01 1.109110143917E+00 -2.625871228027E+00
H -4.421262776669E+00 2.352695994122E+00 -1.609393232482E+00
H 1.530004358785E+00 2.849317489550E+00 -8.194425705282E-02
H 7.481271494240E+00 2.441300814360E+00 1.471521441000E+00
H -8.388774200306E+00 1.258188380019E+00 2.557789478808E+00
H -2.437507064851E+00 -3.243899750446E-01 2.831977429572E+00
H 3.513760070603E+00 -1.803976805061E+00 2.207032556243E+00
H 9.465027206058E+00 -2.710813745762E+00 8.813704404540E-01
H -6.405018488488E+00 -2.756986475878E+00 -7.241205627136E-01
H 4.543057161305E-01 -8.958770993066E-01 2.705974365024E+00
H 6.405572851585E+00 -2.216619967495E+00 1.792062767018E+00
H -9.464472842960E+00 -2.833601657891E+00 3.091839025945E-01
H -3.513205707506E+00 -2.550934843180E+00 -1.271858666314E+00
H 2.438061427949E+00 -1.458364239804E+00 -2.449095095191E+00
H 8.389328563403E+00 9.722670540124E-02 -2.848761135825E+00
H -7.480717131142E+00 1.621948858612E+00 -2.343965644218E+00
H -1.529449995688E+00 2.631713709357E+00 -1.094977622242E+00
H 4.421817139767E+00 2.805928052181E+00 5.016580580537E-01
H 1.037308427522E+01 2.089280064178E+00 1.939020849464E+00
H -5.496961419324E+00 7.093004179462E-01 2.760758221636E+00
H 1.156763400437E+00 -2.279060761659E+00 1.876800109309E+00
H 7.108030535892E+00 -2.931942662580E+00 3.467114491598E-01
H -8.762015158654E+00 -2.653953484249E+00 -1.293455646352E+00
H -2.810748023199E+00 -1.533352826608E+00 -2.522959713267E+00
H 3.140519112255E+00 7.407651932761E-02 -2.951441897602E+00
H 9.091786247710E+00 1.657987093776E+00 -2.442862133340E+00
H -6.778259446836E+00 2.715498480728E+00 -1.158690902182E+00
H -8.269923113812E-01 2.910858286844E+00 4.933565035006E-01

H 5.124274824073E+00 2.182041154029E+00 1.988766705212E+00
H -1.074577087047E+01 7.604413723757E-01 2.852757529973E+00
H -4.794503735018E+00 -9.025931719850E-01 2.811017995588E+00
H -5.719256735954E-01 -2.216719072495E+00 2.175979695570E+00
H 5.379341461859E+00 -3.041246192410E+00 6.321017948441E-01
H -1.049070423269E+01 -2.900199134654E+00 -1.112463959527E+00
H -4.539437097232E+00 -1.838359343473E+00 -2.503830267043E+00
H 1.411830038223E+00 -1.928534499659E-01 -3.100248155992E+00
H 7.363097173677E+00 1.513882051268E+00 -2.712359160720E+00
H -8.506948520868E+00 2.739970697804E+00 -1.463315296534E+00
H -2.555681385414E+00 3.096138007495E+00 2.503208350101E-01
H 3.395585750041E+00 2.469303376072E+00 1.884481870121E+00
H 9.346852885496E+00 1.058482370010E+00 2.920333226581E+00
H -6.523192809050E+00 -6.883993096509E-01 3.028999417690E+00

PbE0/POB-TZVP optimized geometry, *all*-[-98.4]-$(GeMe_2)_\infty$

Energy (a.u): -4.0973700382183E+04
Unit cell length (Å): 34.76219305

Ge	1.081078499411E-01	-9.870684744272E-02	9.390698693419E-01
Ge	5.596875173625E+00	-3.982741263067E-01	8.561384126136E-01
Ge	1.108564249731E+01	-6.546822237255E-01	6.804310745224E-01
Ge	1.657440982099E+01	-8.401453437623E-01	4.309884715308E-01
Ge	-1.269901590532E+01	-9.345656796043E-01	1.348415801736E-01
Ge	-7.210248581638E+00	-9.277113227805E-01	-1.759174886780E-01
Ge	-1.721481257954E+00	-8.203250492091E-01	-4.676131679904E-01
Ge	3.767286065731E+00	-6.240438279013E-01	-7.086357047850E-01
Ge	9.256053389415E+00	-3.601377748027E-01	-8.728665673504E-01
Ge	1.474482071310E+01	-5.720520569094E-02	-9.425087934230E-01
Ge	-1.452860501322E+01	2.519264350877E-01	-9.100155671976E-01
Ge	-9.039837689533E+00	5.337579375832E-01	-7.789080339198E-01
Ge	-3.551070365848E+00	7.577484854338E-01	-5.633937291635E-01
Ge	1.937696957836E+00	8.996252272084E-01	-2.868269718979E-01
Ge	7.426464281520E+00	9.440136164914E-01	2.082193835195E-02
Ge	1.291523160520E+01	8.861034825470E-01	3.262144684956E-01
Ge	-1.635819412111E+01	7.321702869565E-01	5.962565992388E-01
Ge	-1.086942679743E+01	4.988950799818E-01	8.016850755801E-01
Ge	-5.380659473743E+00	2.115568499362E-01	9.202385345567E-01
C	7.204481726510E-01	-1.652404305162E+00	1.971348613612E+00
C	6.209215496335E+00	-2.202968330540E+00	1.328000707359E+00
C	1.169798282002E+01	-2.514806554728E+00	5.407433184100E-01
C	1.718675014370E+01	-2.554126467467E+00	-3.051119995860E-01
C	-1.208667558261E+01	-2.316667146101E+00	-1.117903698126E+00
C	-6.597908258928E+00	-1.828160992660E+00	-1.809553184912E+00
C	-1.109140935244E+00	-1.141545228824E+00	-2.305109506001E+00
C	4.379626388440E+00	-3.312253265454E-01	-2.550871444656E+00
C	9.868393712125E+00	5.149879793547E-01	-2.520206881434E+00
C	1.535716103581E+01	1.305394346830E+00	-2.216438797570E+00
C	-1.391626469051E+01	1.954340981546E+00	-1.672485178397E+00
C	-8.427497366823E+00	2.391504446186E+00	-9.472918388640E-01
C	-2.938730043139E+00	2.569511296068E+00	-1.194447298425E-01
C	2.550037280546E+00	2.469071726945E+00	7.213460690334E-01
C	8.038804604230E+00	2.101069924612E+00	1.483967828492E+00
C	1.352757192791E+01	1.505384594488E+00	2.085778647600E+00
C	-1.574585379840E+01	7.465674851034E-01	2.461562986051E+00
C	-1.025708647472E+01	-9.315179548069E-02	2.570598779877E+00
C	-4.768319151033E+00	-9.227766336254E-01	2.401070308955E+00
C	-5.041341377529E-01	1.206347202152E+00	2.271919266108E+00
C	4.984633185931E+00	4.032930034915E-01	2.540520709852E+00

C 1.047340050962E+01 -4.434642498330E-01 2.533817314443E+00
C 1.596216783330E+01 -1.242165270631E+00 2.252535496788E+00
C -1.331125789302E+01 -1.906258410177E+00 1.727156506366E+00
C -7.822490569332E+00 -2.363778872332E+00 1.014613308885E+00
C -2.333723245648E+00 -2.565147215863E+00 1.921210160392E-01
C 3.155044078037E+00 -2.488542056194E+00 -6.511905699596E-01
C 8.643811401721E+00 -2.142264751029E+00 -1.423935553440E+00
C 1.413257872540E+01 -1.563839819427E+00 -2.042375025070E+00
C -1.514084700091E+01 -8.159485779149E-01 -2.439491472019E+00
C -9.652079677227E+00 2.036335276073E-02 -2.572251165364E+00
C -4.163312353542E+00 8.544685981948E-01 -2.426267532353E+00
C 1.325454970142E+00 1.595978912568E+00 -2.017360164792E+00
C 6.814222293826E+00 2.164540147600E+00 -1.389840520808E+00
C 1.230298961751E+01 2.498539871339E+00 -6.117100907962E-01
C -1.697043610881E+01 2.561784031178E+00 2.327086192132E-01
C -1.148166878512E+01 2.347419141063E+00 1.051909739485E+00
C -5.992901461437E+00 1.878674963054E+00 1.757120117421E+00
H -2.111424770228E-02 -1.930219867738E+00 2.721635122808E+00
H 5.467653075982E+00 -2.709348710924E+00 1.947428058267E+00
H 1.095642039967E+01 -3.194877581405E+00 9.621869461530E-01
H 1.644518772335E+01 -3.334191892307E+00 -1.273220514454E-01
H -1.282823800297E+01 -3.112194776360E+00 -1.203033729165E+00
H -7.339470679281E+00 -2.552943065717E+00 -2.148378035337E+00
H -1.850703355597E+00 -1.717040360911E+00 -2.860912245861E+00
H 3.638063968087E+00 -6.950696903728E-01 -3.263422222918E+00
H 9.126831291771E+00 4.022225662342E-01 -3.312289764910E+00
H 1.461559861546E+01 1.455927766664E+00 -3.002219315402E+00
H -1.465782711086E+01 2.351860602528E+00 -2.366811818837E+00
H -9.169059787176E+00 2.992932849231E+00 -1.474923536833E+00
H -3.680292463492E+00 3.309674381582E+00 -4.232044038160E-01
H 1.808474860192E+00 3.267761339800E+00 6.743754930473E-01
H 7.297242183877E+00 2.871735652308E+00 1.698876341225E+00
H 1.278600950756E+01 2.164512847319E+00 2.539277577049E+00
H -1.648741621875E+01 1.222731489446E+00 3.104508686448E+00
H -1.099864889507E+01 1.484482020576E-01 3.333318108255E+00
H -5.509881571386E+00 -9.419217514351E-01 3.200910791273E+00
H 1.651410059396E+00 -1.440394974529E+00 2.500146697153E+00
H 7.140177383080E+00 -2.174146707268E+00 1.896986369274E+00
H 1.262894470676E+01 -2.672295908912E+00 1.088258133507E+00
H -1.664448101955E+01 -2.880860383883E+00 1.616002429102E-01
H -1.115571369587E+01 -2.777238935105E+00 -7.825695414920E-01
H -5.666946372183E+00 -2.372660554406E+00 -1.641935773256E+00
H -1.781790484989E-01 -1.710967587016E+00 -2.323372786729E+00
H 5.310588275185E+00 -8.638647331751E-01 -2.753036307917E+00
H 1.079935559887E+01 7.685126874777E-02 -2.884365627382E+00

H 1.628812292255E+01 1.009239243232E+00 -2.703129175577E+00
H -1.298530280376E+01 1.832260485751E+00 -2.228966734227E+00
H -7.496535480078E+00 2.456727874188E+00 -1.513261161241E+00
H -2.007768156394E+00 2.814970677397E+00 -6.335702607683E-01
H 3.480999167291E+00 2.868167728939E+00 3.147778083141E-01
H 8.969766490975E+00 2.610554302843E+00 1.229014817585E+00
H 1.445853381466E+01 2.070046811110E+00 2.010069001240E+00
H -1.481489191166E+01 1.305217627308E+00 2.573301019177E+00
H -9.326124587973E+00 3.989478610486E-01 2.857675942807E+00
H -3.837357264288E+00 -5.505540962691E-01 2.832377336623E+00
H 8.899181461229E-01 -2.524840786761E+00 1.342260611833E+00
H 6.378685469807E+00 -2.823869256864E+00 4.497187662397E-01
H 1.186745279349E+01 -2.816887676140E+00 -4.915570857814E-01
H 1.735622011718E+01 -2.504652607190E+00 -1.379565100264E+00
H -1.191720560914E+01 -1.920999564562E+00 -2.118075829975E+00
H -6.428438285456E+00 -1.129176411734E+00 -2.627060178175E+00
H -9.396709617718E-01 -2.149894737173E-01 -2.851361793032E+00
H 4.549096361912E+00 7.224949096820E-01 -2.766674114176E+00
H 1.003786368560E+01 1.581685758954E+00 -2.382174365678E+00
H 1.552663100928E+01 2.269476413859E+00 -1.739529061415E+00
H -1.374679471703E+01 2.711334084769E+00 -9.083787917727E-01
H -8.258027393351E+00 2.859376636910E+00 2.120841490709E-02
H -2.769260069667E+00 2.697561362643E+00 9.484973607492E-01
H 2.719507254018E+00 2.243423457755E+00 1.773001900101E+00
H 8.208274577702E+00 1.546175810919E+00 2.405374172618E+00
H 1.369704190139E+01 6.813760235798E-01 2.777086830306E+00
H -1.557638382493E+01 -2.572614285526E-01 2.847859038989E+00
H -1.008761650125E+01 -1.168020613079E+00 2.610021531711E+00
H -4.598849177561E+00 -1.952206640471E+00 2.089347692815E+00
H -6.748222744689E-01 2.190230870500E+00 1.837820523798E+00
H 4.813945049215E+00 1.474818772053E+00 2.449409139647E+00
H 1.030271237290E+01 5.995871754834E-01 2.795566268716E+00
H 1.579147969658E+01 -3.406189951037E-01 2.838780414889E+00
H -1.348194602973E+01 -1.243913812323E+00 2.574368654893E+00
H -7.993178706048E+00 -2.012411266666E+00 2.030984105694E+00
H -2.504411382364E+00 -2.562832734487E+00 1.267510914677E+00
H 2.984355941321E+00 -2.835531509079E+00 3.666832485973E-01
H 8.473123265005E+00 -2.800956446859E+00 -5.738802371451E-01
H 1.396189058869E+01 -2.462854292303E+00 -1.452254894524E+00
H -1.531153513763E+01 -1.857863660055E+00 -2.173255200024E+00
H -9.822767813943E+00 -1.051544672515E+00 -2.658749583073E+00
H -4.334000490258E+00 -1.312745033114E-01 -2.856127194045E+00
H 1.154766833426E+00 8.032212952599E-01 -2.743999106163E+00
H 6.643534157110E+00 1.650675603227E+00 -2.334516137596E+00
H 1.213230148079E+01 2.319253596714E+00 -1.672052121769E+00

H -1.714112424552E+01 2.736504476069E+00 -8.283953139874E-01
H -1.165235692184E+01 2.857212634201E+00 1.050309799426E-01
H -6.163589598153E+00 2.668297469195E+00 1.027075537472E+00
H -1.434428756205E+00 8.884161055873E-01 2.745992081957E+00
H 4.054338567479E+00 -5.134290098270E-02 2.885674894605E+00
H 9.543105891164E+00 -9.855381075640E-01 2.712650056564E+00
H 1.503187321485E+01 -1.812934967991E+00 2.245667493791E+00
H -1.424155251147E+01 -2.443872194053E+00 1.535332012945E+00
H -8.752785187784E+00 -2.809977947304E+00 6.586194853655E-01
H -3.264017864099E+00 -2.871578988665E+00 -2.894646829878E-01
H 2.224749459585E+00 -2.621999889465E+00 -1.206180861432E+00
H 7.713516783269E+00 -2.088286417721E+00 -1.992188627716E+00
H 1.320228410695E+01 -1.328274709515E+00 -2.562311844195E+00
H -1.607114161936E+01 -4.243238262272E-01 -2.854768813991E+00
H -1.058237429568E+01 5.256091276948E-01 -2.837867286488E+00
H -5.093606971994E+00 1.418584176965E+00 -2.513438804447E+00
H 3.951603516900E-01 2.157833619060E+00 -1.916640227923E+00
H 5.883927675374E+00 2.663248306291E+00 -1.112143942966E+00
H 1.137269499906E+01 2.880058714980E+00 -1.871296050971E-01
H 1.686146232274E+01 2.784770073186E+00 7.581631290989E-01
H -1.241196340357E+01 2.387708383802E+00 1.621297124144E+00
H -6.923196079889E+00 1.731901441921E+00 2.308738418771E+00
H 2.379565934184E-01 1.323015639313E+00 3.062949165099E+00
H 5.726723917103E+00 2.567930345932E-01 3.326572606638E+00
H 1.121549124079E+01 -8.372570799792E-01 3.229710289155E+00
H 1.670425856447E+01 -1.840577398554E+00 2.782858747723E+00
H -1.256916716184E+01 -2.644442596494E+00 2.034441280474E+00
H -7.080399838161E+00 -3.161741406350E+00 1.065560532876E+00
H -1.591632514476E+00 -3.336416475354E+00 -1.879023233457E-02
H 3.897134809208E+00 -3.149539049419E+00 -1.101104784311E+00
H 9.385902132892E+00 -2.621360197345E+00 -2.064097547506E+00
H 1.487466945658E+01 -1.809116293295E+00 -2.803413313656E+00
H -1.439875626974E+01 -8.008265675348E-01 -3.238935747831E+00
H -8.909988946055E+00 2.942451429225E-01 -3.323469236463E+00
H -3.421221622371E+00 1.357430826460E+00 -3.047853264385E+00
H 2.067545701313E+00 2.273517817242E+00 -2.441955098795E+00
H 7.556313024997E+00 2.943233875261E+00 -1.571433207414E+00
H 1.304508034868E+01 3.294004873917E+00 -5.306221447101E-01
H -1.622834537763E+01 3.287819332732E+00 5.676900608236E-01
H -1.073957805395E+01 2.925347551073E+00 1.604484239648E+00
H -5.250810730266E+00 2.245868970810E+00 2.467407654969E+00

PbE0/POB-TZVP optimized geometry, *all*-[86.5]-$(GeMe_2)_\infty$

Energy (a.u): -5.1756281009401E+04
Unit cell length (Å): 41.83809032

Ge	-9.148577433602E-06	-1.030412069579E+00	2.213042936824E-01
Ge	1.220276719476E+01	-1.052579395694E+00	-5.292673517406E-02
Ge	-1.743254678191E+01	-1.003015175463E+00	-3.235508944940E-01
Ge	-5.229770438577E+00	-8.850971285843E-01	-5.721255950473E-01
Ge	6.973005904756E+00	-7.068611750850E-01	-7.817108817803E-01
Ge	1.917578224809E+01	-4.804538006470E-01	-9.380238637584E-01
Ge	-1.045953172858E+01	-2.213042936824E-01	-1.030412069579E+00
Ge	1.743244614756E+00	5.292673517406E-02	-1.052579395694E+00
Ge	1.394602095809E+01	3.235508944940E-01	-1.003015175463E+00
Ge	-1.568929301858E+01	5.721255950473E-01	-8.850971285843E-01
Ge	-3.486516675244E+00	7.817108817803E-01	-7.068611750850E-01
Ge	8.716259668089E+00	9.380238637584E-01	-4.804538006470E-01
Ge	2.091903601142E+01	1.030412069579E+00	-2.213042936824E-01
Ge	-8.716277965244E+00	1.052579395694E+00	5.292673517406E-02
Ge	3.486498378089E+00	1.003015175463E+00	3.235508944940E-01
Ge	1.568927472142E+01	8.850971285843E-01	5.721255950473E-01
Ge	-1.394603925524E+01	7.068611750850E-01	7.817108817803E-01
Ge	-1.743262911911E+00	4.804538006470E-01	9.380238637584E-01
Ge	1.045951343142E+01	2.213042936824E-01	1.030412069579E+00
Ge	-1.917580054524E+01	-5.292673517406E-02	1.052579395694E+00
Ge	-6.973024201911E+00	-3.235508944940E-01	1.003015175463E+00
Ge	5.229752141423E+00	-5.721255950473E-01	8.850971285843E-01
Ge	1.743252848476E+01	-7.817108817803E-01	7.068611750850E-01
Ge	-1.220278549191E+01	-9.380238637584E-01	4.804538006470E-01
C	-7.534801547700E-01	-2.484873209780E+00	-8.614231525438E-01
C	1.144929618856E+01	-2.177250490610E+00	-1.475203381761E+00
C	-1.818601778810E+01	-1.721251748581E+00	-1.988450938401E+00
C	-5.983241444770E+00	-1.147952544389E+00	-2.366188849659E+00
C	6.219534898563E+00	-4.964222713790E-01	-2.582674901125E+00
C	1.842231124190E+01	1.889383590493E-01	-2.623155926151E+00
C	-1.121300273477E+01	8.614231525438E-01	-2.484873209780E+00
C	9.897736085633E-01	1.475203381761E+00	-2.177250490610E+00
C	1.319254995190E+01	1.988450938401E+00	-1.721251748581E+00
C	-1.644276402477E+01	2.366188849659E+00	-1.147952544389E+00
C	-4.239987681437E+00	2.582674901125E+00	-4.964222713790E-01
C	7.962788661897E+00	2.623155926151E+00	1.889383590493E-01
C	2.016556500523E+01	2.484873209780E+00	8.614231525438E-01
C	-9.469748971437E+00	2.177250490610E+00	1.475203381761E+00
C	2.733027371897E+00	1.721251748581E+00	1.988450938401E+00
C	1.493580371523E+01	1.147952544389E+00	2.366188849659E+00

C -1.469951026144E+01 4.964222713790E-01 2.582674901125E+00
C -2.496733918103E+00 -1.889383590493E-01 2.623155926151E+00
C 9.706042425230E+00 -8.614231525438E-01 2.484873209780E+00
C -1.992927155144E+01 -1.475203381761E+00 2.177250490610E+00
C -7.726495208103E+00 -1.988450938401E+00 1.721251748581E+00
C 4.476281135230E+00 -2.366188849659E+00 1.147952544389E+00
C 1.667905747856E+01 -2.582674901125E+00 4.964222713790E-01
C -1.295625649810E+01 -2.623155926151E+00 -1.889383590493E-01
C 7.534824355275E-01 -1.911892685994E+00 1.805834995464E+00
C 1.295625877886E+01 -2.314131011633E+00 1.249468420808E+00
C -1.667905519781E+01 -2.558665133112E+00 6.079526381178E-01
C -4.476278854473E+00 -2.628830454164E+00 -7.499411217075E-02
C 7.726497488861E+00 -2.519845324112E+00 -7.528301376485E-01
C 1.992927383219E+01 -2.239136899463E+00 -1.379362033356E+00
C -9.706040144473E+00 -1.805834995464E+00 -1.911892685994E+00
C 2.496736198861E+00 -1.249468420808E+00 -2.314131011633E+00
C 1.469951254219E+01 -6.079526381178E-01 -2.558665133112E+00
C -1.493580143447E+01 7.499411217075E-02 -2.628830454164E+00
C -2.733025091139E+00 7.528301376485E-01 -2.519845324112E+00
C 9.469751252194E+00 1.379362033356E+00 -2.239136899463E+00
C -2.016556272447E+01 1.911892685994E+00 -1.805834995464E+00
C -7.962786381139E+00 2.314131011633E+00 -1.249468420808E+00
C 4.239989962194E+00 2.558665133112E+00 -6.079526381178E-01
C 1.644276630553E+01 2.628830454164E+00 7.499411217075E-02
C -1.319254767114E+01 2.519845324112E+00 7.528301376485E-01
C -9.897713278058E-01 2.239136899463E+00 1.379362033356E+00
C 1.121300501553E+01 1.805834995464E+00 1.911892685994E+00
C -1.842230896114E+01 1.249468420808E+00 2.314131011633E+00
C -6.219532617806E+00 6.079526381178E-01 2.558665133112E+00
C 5.983243725527E+00 -7.499411217075E-02 2.628830454164E+00
C 1.818602006886E+01 -7.528301376485E-01 2.519845324112E+00
C -1.144929390781E+01 -1.379362033356E+00 2.239136899463E+00
H -1.461380532870E+00 -3.073450856126E+00 -2.772662102204E-01
H 1.074139581046E+01 -2.896963781994E+00 -1.063286208961E+00
H -1.889391816620E+01 -2.523053413578E+00 -1.776845009725E+00
H -6.691141822870E+00 -1.977201124570E+00 -2.369314759451E+00
H 5.511634520463E+00 -1.296605846401E+00 -2.800319623798E+00
H 1.771441086380E+01 -5.276490225429E-01 -3.040487333531E+00
H -1.192090311287E+01 2.772662102204E-01 -3.073450856126E+00
H 2.818732304630E-01 1.063286208961E+00 -2.896963781994E+00
H 1.248464957380E+01 1.776845009725E+00 -2.523053413578E+00
H -1.715066440287E+01 2.369314759451E+00 -1.977201124570E+00
H -4.947888059537E+00 2.800319623798E+00 -1.296605846401E+00
H 7.254888283796E+00 3.040487333531E+00 -5.276490225429E-01
H 1.945766462713E+01 3.073450856126E+00 2.772662102204E-01

H -1.017764934954E+01 2.896963781994E+00 1.063286208961E+00
H 2.025126993796E+00 2.523053413578E+00 1.776845009725E+00
H 1.422790333713E+01 1.977201124570E+00 2.369314759451E+00
H -1.540741063954E+01 1.296605846401E+00 2.800319623798E+00
H -3.204634296204E+00 5.276490225429E-01 3.040487333531E+00
H 8.998142047130E+00 -2.772662102204E-01 3.073450856126E+00
H -2.063717192954E+01 -1.063286208961E+00 2.896963781994E+00
H -8.434395586204E+00 -1.776845009725E+00 2.523053413578E+00
H 3.768380757130E+00 -2.369314759451E+00 1.977201124570E+00
H 1.597115710046E+01 -2.800319623798E+00 1.296605846401E+00
H -1.366415687620E+01 -3.040487333531E+00 5.276490225429E-01
H 3.231019185023E-02 -3.160481160238E+00 -1.202123852396E+00
H 1.223508653518E+01 -2.741657828602E+00 -1.979155191385E+00
H -1.740022744148E+01 -2.135995046750E+00 -2.621310374789E+00
H -5.197451098150E+00 -1.384767732361E+00 -3.084827588072E+00
H 7.005325245184E+00 -5.391707854488E-01 -3.338118899146E+00
H 1.920810158852E+01 3.431697594701E-01 -3.363922923746E+00
H -1.042721238815E+01 1.202123852396E+00 -3.160481160238E+00
H 1.775563955184E+00 1.979155191385E+00 -2.741657828602E+00
H 1.397834029852E+01 2.621310374789E+00 -2.135995046750E+00
H -1.565697367815E+01 3.084827588072E+00 -1.384767732361E+00
H -3.454197334816E+00 3.338118899146E+00 -5.391707854489E-01
H 8.748579008517E+00 3.363922923746E+00 3.431697594701E-01
H -2.088673496815E+01 3.160481160238E+00 1.202123852396E+00
H -8.683958624816E+00 2.741657828602E+00 1.979155191385E+00
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H -1.391371991482E+01 5.391707854489E-01 3.338118899146E+00
H -1.710943571483E+00 -3.431697594701E-01 3.363922923746E+00
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H -1.914348120482E+01 -1.979155191385E+00 2.741657828602E+00
H -6.940704861483E+00 -2.621310374789E+00 2.135995046750E+00
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H -1.217046615148E+01 -3.363922923746E+00 -3.431697594701E-01
H -1.275885826036E+00 -2.123381384559E+00 -1.747249157608E+00
H 1.092689051730E+01 -1.598807559879E+00 -2.237284628635E+00
H -1.870842345937E+01 -9.652776421471E-01 -2.574852849509E+00
H -6.505647116036E+00 -2.659656482998E-01 -2.736949103834E+00
H 5.697129227297E+00 4.514714649500E-01 -2.712526799755E+00
H 1.789990557063E+01 1.138141543955E+00 -2.503250276935E+00
H -1.173540840604E+01 1.747249157608E+00 -2.123381384559E+00
H 4.673679372971E-01 2.237284628635E+00 -1.598807559879E+00
H 1.267014428063E+01 2.574852849509E+00 -9.652776421471E-01
H -1.696516969604E+01 2.736949103834E+00 -2.659656482998E-01

H -4.762393352703E+00 2.712526799755E+00 4.514714649500E-01
H 7.440382990630E+00 2.503250276935E+00 1.138141543955E+00
H 1.964315933396E+01 2.123381384559E+00 1.747249157608E+00
H -9.992154642703E+00 1.598807559879E+00 2.237284628635E+00
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H 1.441339804396E+01 2.659656482999E-01 2.736949103834E+00
H -1.522191593270E+01 -4.514714649500E-01 2.712526799755E+00
H -3.019139589370E+00 -1.138141543955E+00 2.503250276935E+00
H 9.183636753964E+00 -1.747249157608E+00 2.123381384559E+00
H -2.045167722270E+01 -2.237284628635E+00 1.598807559879E+00
H -8.248900879369E+00 -2.574852849509E+00 9.652776421471E-01
H 3.953875463964E+00 -2.736949103834E+00 2.659656482998E-01
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H 1.275171068039E+00 -1.218366131523E+00 2.465492593171E+00
H 1.347794741137E+01 -1.814967750986E+00 2.066146611522E+00
H -1.615736656529E+01 -2.287882317595E+00 1.525996152767E+00
H -3.954590221961E+00 -2.604881485164E+00 8.818515780285E-01
H 8.248186121372E+00 -2.744362284290E+00 1.776102755760E-01
H 2.045096246471E+01 -2.696819329014E+00 -5.387348736421E-01
H -9.184351511961E+00 -2.465492593171E+00 -1.218366131523E+00
H 3.018424831372E+00 -2.066146611522E+00 -1.814967750986E+00
H 1.522120117471E+01 -1.525996152767E+00 -2.287882317595E+00
H -1.441411280196E+01 -8.818515780285E-01 -2.604881485164E+00
H -2.211336458628E+00 -1.776102755760E-01 -2.744362284290E+00
H 9.991439884705E+00 5.387348736421E-01 -2.696819329014E+00
H -1.964387409196E+01 1.218366131523E+00 -2.465492593171E+00
H -7.441097748628E+00 1.814967750986E+00 -2.066146611522E+00
H 4.761678594705E+00 2.287882317595E+00 -1.525996152767E+00
H 1.696445493804E+01 2.604881485164E+00 -8.818515780285E-01
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H 1.173469364804E+01 2.465492593171E+00 1.218366131523E+00
H -1.790062032863E+01 2.066146611522E+00 1.814967750986E+00
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H -1.092760527529E+01 -5.387348736421E-01 2.696819329014E+00
H 1.462016527476E+00 -2.687897795040E+00 1.515004569213E+00
H 1.366479287081E+01 -2.988421934584E+00 7.677028997034E-01
H -1.597052110586E+01 -3.085290057887E+00 -3.191645373204E-02
H -3.767744762524E+00 -2.971900762428E+00 -8.293607535900E-01
H 8.435031580809E+00 -2.655981341308E+00 -1.570285488674E+00
H 2.063780792414E+01 -2.159061180994E+00 -2.204197862725E+00
H -8.997506052524E+00 -1.515004569213E+00 -2.687897795040E+00

H 3.205270290809E+00 -7.677028997034E-01 -2.988421934584E+00
H 1.540804663414E+01 3.191645373204E-02 -3.085290057887E+00
H -1.422726734252E+01 8.293607535900E-01 -2.971900762428E+00
H -2.024490999191E+00 1.570285488674E+00 -2.655981341308E+00
H 1.017828534414E+01 2.204197862725E+00 -2.159061180994E+00
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H -7.254252289191E+00 2.988421934584E+00 -7.677028997034E-01
H 4.948524054142E+00 3.085290057887E+00 3.191645373204E-02
H 1.715130039748E+01 2.971900762428E+00 8.293607535900E-01
H -1.248401357919E+01 2.655981341308E+00 1.570285488674E+00
H -2.812372358576E-01 2.159061180994E+00 2.204197862725E+00
H 1.192153910748E+01 1.515004569213E+00 2.687897795040E+00
H -1.771377486919E+01 7.677028997034E-01 2.988421934584E+00
H -5.510998525858E+00 -3.191645373204E-02 3.085290057887E+00
H 6.691777817476E+00 -8.293607535900E-01 2.971900762428E+00
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H -1.074075981586E+01 -2.204197862725E+00 2.159061180994E+00
H -3.222456063828E-02 -2.388680344272E+00 2.393471225741E+00
H 1.217055178270E+01 -2.926763972408E+00 1.693679705663E+00
H -1.746476219397E+01 -3.265393472531E+00 8.784667125828E-01
H -5.261985850638E+00 -3.381491803818E+00 3.387664774591E-03
H 6.940790492695E+00 -3.267147056855E+00 -8.719222467896E-01
H 1.914356683603E+01 -2.930151637183E+00 -1.687812098155E+00
H -1.049174714064E+01 -2.393471225741E+00 -2.388680344272E+00
H 1.711029202695E+00 -1.693679705663E+00 -2.926763972408E+00
H 1.391380554603E+01 -8.784667125828E-01 -3.265393472531E+00
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H -3.518732087305E+00 8.719222467896E-01 -3.267147056855E+00
H 8.684044256028E+00 1.687812098155E+00 -2.930151637183E+00
H 2.088682059936E+01 2.388680344272E+00 -2.393471225741E+00
H -8.748493377305E+00 2.926763972408E+00 -1.693679705663E+00
H 3.454282966028E+00 3.265393472531E+00 -8.784667125828E-01
H 1.565705930936E+01 3.381491803818E+00 -3.387664774593E-03
H -1.397825466730E+01 3.267147056855E+00 8.719222467896E-01
H -1.775478323972E+00 2.930151637183E+00 1.687812098155E+00
H 1.042729801936E+01 2.393471225741E+00 2.388680344272E+00
H -1.920801595730E+01 1.693679705663E+00 2.926763972408E+00
H -7.005239613972E+00 8.784667125828E-01 3.265393472531E+00
H 5.197536729362E+00 3.387664774591E-03 3.381491803818E+00
H 1.740031307270E+01 -8.719222467896E-01 3.267147056855E+00
H -1.223500090397E+01 -1.687812098155E+00 2.930151637183E+00

PbE0/POB-TZVP optimized geometry, *all*-[-75.3]-$(GeMe_2)_\infty$

Energy (a.u): -4.9599757822434E+04
Unit cell length (Å): 40.02214982

Ge	1.193210453289E-01	-1.195417854909E-01	1.137858094622E+00
Ge	-6.841052836410E+00	-4.220992917735E-01	1.063411242116E+00
Ge	-1.380142671815E+01	-6.933516245610E-01	9.100960425657E-01
Ge	1.926034922011E+01	-9.131812392275E-01	6.892831829503E-01
Ge	1.229997533837E+01	-1.065284378907E+00	4.173493429162E-01
Ge	5.339601456633E+00	-1.138380249554E+00	1.144626113642E-01
Ge	-1.620772425106E+00	-1.127047664835E+00	-1.969132884411E-01
Ge	-8.581146306845E+00	-1.032127110715E+00	-4.936850304610E-01
Ge	-1.554152018858E+01	-8.606584104613E-01	-7.538424122304E-01
Ge	1.752025574968E+01	-6.253586131535E-01	-9.580907508842E-01
Ge	1.055988186794E+01	-3.436788283334E-01	-1.091281881518E+00
Ge	3.599507986198E+00	-3.650995704179E-02	-1.143537627283E+00
Ge	-3.360865895541E+00	2.733666907416E-01	-1.110982418568E+00
Ge	-1.032123977728E+01	5.629689816422E-01	-9.960307262750E-01
Ge	-1.728161365902E+01	8.108184385860E-01	-8.072079915512E-01
Ge	1.578016227924E+01	9.985332011875E-01	-5.585183328248E-01
Ge	8.819788397503E+00	1.112191324242E+00	-2.684059244042E-01
Ge	1.859414515764E+00	1.143363304715E+00	4.161292355401E-02
Ge	-5.100959365975E+00	1.089737259416E+00	3.485455313387E-01
Ge	-1.206133324771E+01	9.552903868020E-01	6.296281115538E-01
Ge	-1.902170712945E+01	7.499939963620E-01	8.640140550918E-01
Ge	1.404006880881E+01	4.890739822059E-01	1.034320028765E+00
Ge	7.079694927068E+00	1.918815881543E-01	1.127915217604E+00
C	9.111895496756E-01	-1.585675848883E+00	2.177303545739E+00
C	-6.049184332063E+00	-2.114304153488E+00	1.668752999865E+00
C	-1.300955821380E+01	-2.486124191328E+00	1.036438678029E+00
C	-1.996993209554E+01	-2.673559771157E+00	3.272564408343E-01
C	1.309184384272E+01	-2.662709653482E+00	-4.061969094783E-01
C	6.131469960980E+00	-2.454378541895E+00	-1.109524493242E+00
C	-8.289039207591E-01	-2.064017401890E+00	-1.730563721079E+00
C	-7.789277802498E+00	-1.520577533438E+00	-2.223254954526E+00
C	-1.474965168424E+01	-8.643633855100E-01	-2.551057538710E+00
C	1.831212425402E+01	-1.440433594784E-01	-2.689659855560E+00
C	1.135175037228E+01	5.869597035712E-01	-2.628782405298E+00
C	4.391376490545E+00	1.274430650569E+00	-2.372940189914E+00
C	-2.568997391194E+00	1.867382906346E+00	-1.941107856123E+00
C	-9.529371272933E+00	2.321839914668E+00	-1.365312432622E+00
C	-1.648974515467E+01	2.604096678230E+00	-6.882580318815E-01
C	1.657203078359E+01	2.693219504117E+00	3.984131851258E-02
C	9.611656901850E+00	2.582598560043E+00	7.649858205744E-01

C 2.651283020110E+00 2.280438095373E+00 1.433394823902E+00
C -4.309090861629E+00 1.809147969480E+00 1.995495490485E+00
C -1.126946474337E+01 1.203681614991E+00 2.409599385323E+00
C -1.822983862511E+01 5.089437015953E-01 2.644994316936E+00
C 1.483193731315E+01 -2.235402378851E-01 2.684222120106E+00
C 7.871563431415E+00 -9.394452205502E-01 2.524373448126E+00
C -6.724213792837E-01 1.098397613524E+00 2.459526737113E+00
C -7.632795261023E+00 3.940936781964E-01 2.664664943436E+00
C -1.459316914276E+01 -3.394383823845E-01 2.672177140935E+00
C 1.846860679550E+01 -1.047795850971E+00 2.481506184287E+00
C 1.150823291376E+01 -1.678443094638E+00 2.106793266087E+00
C 4.547859032021E+00 -2.184607892342E+00 1.575829129279E+00
C -2.412514849718E+00 -2.528750316588E+00 9.279929548908E-01
C -9.372888731458E+00 -2.685346898114E+00 2.113317883237E-01
C -1.633326261320E+01 -2.642783584853E+00 -5.210028902048E-01
C 1.672851332506E+01 -2.404217103033E+00 -1.214697167796E+00
C 9.768139443325E+00 -1.987340837243E+00 -1.818302913322E+00
C 2.807765561586E+00 -1.423072593033E+00 -2.287053449950E+00
C -4.152608320153E+00 -7.532615647228E-01 -2.586183694767E+00
C -1.111298220189E+01 -2.758457209904E-02 -2.693508525947E+00
C -1.807335608363E+01 7.001382420463E-01 -2.601068151739E+00
C 1.498841985463E+01 1.375935005698E+00 -2.315718451812E+00
C 8.028045972890E+00 1.949684964462E+00 -1.858622508021E+00
C 1.067672091151E+00 2.378835708626E+00 -1.263681035442E+00
C -5.892701790588E+00 2.631559090731E+00 -5.750181214202E-01
C -1.285307567233E+01 2.689111773658E+00 1.562912561343E-01
C -1.981344955407E+01 2.547225338200E+00 8.760092262062E-01
C 1.324832638419E+01 2.216422852189E+00 1.530757599446E+00
C 6.287952502455E+00 1.721238422691E+00 2.071976684285E+00
H 1.608719951249E-01 -2.056166417883E+00 2.813887688354E+00
H -6.799501886614E+00 -2.739096002160E+00 2.154794039265E+00
H -1.375987576835E+01 -3.218879366487E+00 1.335889173810E+00
H 1.930190016991E+01 -3.459933173595E+00 4.179075196205E-01
H 1.234152628817E+01 -3.444379565359E+00 -5.310684234999E-01
H 5.381152406429E+00 -3.173372081748E+00 -1.440657451126E+00
H -1.579221475310E+00 -2.667010108045E+00 -2.243399506171E+00
H -8.539595357049E+00 -1.962848195388E+00 -2.879758882713E+00
H -1.549996923879E+01 -1.113110811511E+00 -3.302539716945E+00
H 1.756180669947E+01 -1.808190908886E-01 -3.480386288484E+00
H 1.060143281773E+01 7.648831545131E-01 -3.400108530715E+00
H 3.641058935995E+00 1.653857515452E+00 -3.067660277684E+00
H -3.319314945745E+00 2.420172830365E+00 -2.507697695470E+00
H -1.027968882748E+01 3.006994998003E+00 -1.761750647136E+00
H -1.724006270922E+01 3.370802102727E+00 -8.851426127763E-01
H 1.582171322904E+01 3.484612235885E+00 5.711239991449E-02

H 8.861339347299E+00 3.339984620547E+00 9.951316471755E-01
H 1.900965465560E+00 2.947645625316E+00 1.859346532590E+00
H -5.059408416179E+00 2.336693238637E+00 2.585662191626E+00
H -1.201978229792E+01 1.552439004109E+00 3.120211114527E+00
H -1.898015617966E+01 6.530474705819E-01 3.423348253080E+00
H 1.408161975860E+01 -2.947776063450E-01 3.472591312478E+00
H 7.121245876864E+00 -1.220740376727E+00 3.264288160278E+00
H 1.709967958213E+00 -1.224554505927E+00 2.826065815906E+00
H -5.250405923527E+00 -1.941608135265E+00 2.390886777514E+00
H -1.221077980527E+01 -2.514661571477E+00 1.778386604412E+00
H -1.917115368700E+01 -2.901214062744E+00 1.033991632439E+00
H 1.389062225126E+01 -3.072596779148E+00 2.129102312849E-01
H 6.930248369517E+00 -3.016099048638E+00 -6.239617477242E-01
H -3.012551222226E-02 -2.735911049425E+00 -1.414557338340E+00
H -6.990499393961E+00 -2.252813043637E+00 -2.100241682340E+00
H -1.395087327570E+01 -1.602634200336E+00 -2.630160708727E+00
H 1.911090266256E+01 -8.335953099597E-01 -2.965012747533E+00
H 1.215052878082E+01 -2.732468888488E-03 -3.079963354885E+00
H 5.190154899082E+00 8.283330269000E-01 -2.966487170100E+00
H -1.770218982657E+00 1.597964851455E+00 -2.633000202684E+00
H -8.730592864396E+00 2.249082933180E+00 -2.104235655410E+00
H -1.569096674614E+01 2.733396822621E+00 -1.419409575811E+00
H 1.737080919213E+01 3.014987174186E+00 -6.293123813419E-01
H 1.041043531039E+01 3.072969719691E+00 2.074580335392E-01
H 3.450061428647E+00 2.903044158987E+00 1.028842235130E+00
H -3.510312453092E+00 2.517813093555E+00 1.773921914781E+00
H -1.047068633483E+01 1.945847349202E+00 2.387437921166E+00
H -1.743106021657E+01 1.229567008618E+00 2.823888578740E+00
H 1.563071572169E+01 4.220953078997E-01 3.050904338859E+00
H 8.670341839952E+00 -4.166812708481E-01 3.051648481123E+00
H 1.331330228430E+00 -2.364334285376E+00 1.540942896863E+00
H -5.629043653309E+00 -2.692399774569E+00 8.459107980749E-01
H -1.258941753505E+01 -2.820782289391E+00 8.814136517796E-02
H -1.954979141679E+01 -2.739960286029E+00 -6.761651095543E-01
H 1.351198452147E+01 -2.455927962737E+00 -1.390323511360E+00
H 6.551610639734E+00 -1.989750697572E+00 -2.001367978636E+00
H -4.087632420047E-01 -1.376002725671E+00 -2.463980138585E+00
H -7.369137123744E+00 -6.602029264013E-01 -2.743850163615E+00
H -1.432951100548E+01 1.045611036925E-01 -2.820221374288E+00
H 1.873226493278E+01 8.615703150606E-01 -2.687429667285E+00
H 1.177189105104E+01 1.554680797583E+00 -2.355323596032E+00
H 4.811517169300E+00 2.132487717539E+00 -1.848533948550E+00
H -2.148856712439E+00 2.552137778968E+00 -1.204646994584E+00
H -9.109230594179E+00 2.782507456585E+00 -4.714168839227E-01
H -1.606960447592E+01 2.806511285271E+00 2.967760604301E-01

H 1.699217146234E+01 2.622369010863E+00 1.042958482041E+00
H 1.003179758060E+01 2.243737623460E+00 1.711789444256E+00
H 3.071423698865E+00 1.698698480941E+00 2.253664814307E+00
H -3.888950182874E+00 1.027674643119E+00 2.628396174911E+00
H -1.084932406461E+01 2.804328783162E-01 2.808191415334E+00
H -1.780969794635E+01 -4.876073101766E-01 2.779715945103E+00
H 1.525207799191E+01 -1.219483895129E+00 2.545081659578E+00
H 8.291704110169E+00 -1.860916938347E+00 2.121690310335E+00
H -1.092861860411E+00 1.992243422153E+00 1.999053267409E+00
H -8.053235742150E+00 1.379027514878E+00 2.462423792173E+00
H -1.501360962389E+01 6.635354454560E-01 2.743167609111E+00
H 1.804816631437E+01 -1.011680124830E-01 2.820463233637E+00
H 1.108779243263E+01 -8.583683017490E-01 2.688578002886E+00
H 4.127418550893E+00 -1.551907340848E+00 2.357293241087E+00
H -2.832955330846E+00 -2.130348511980E+00 1.851178823495E+00
H -9.793329212585E+00 -2.550791479674E+00 1.207770941144E+00
H -1.675370309432E+01 -2.782053912416E+00 4.747882132729E-01
H 1.630807284394E+01 -2.806984133523E+00 -2.934073843651E-01
H 9.347698962198E+00 -2.623733182545E+00 -1.039842298554E+00
H 2.387325080459E+00 -2.245891944198E+00 -1.709156866421E+00
H -4.573048801280E+00 -1.701483174622E+00 -2.251711088379E+00
H -1.153342268302E+01 -1.030883181752E+00 -2.627266199804E+00
H -1.849379656476E+01 -2.838272992683E-01 -2.807968996132E+00
H 1.456797937350E+01 4.842787555789E-01 -2.780417577621E+00
H 7.607605491763E+00 1.216468070553E+00 -2.546655306942E+00
H 6.472316100238E-01 1.858437513705E+00 -2.124019262320E+00
H -6.313142271715E+00 2.362575148251E+00 -1.543854425753E+00
H -1.327351615345E+01 2.691491392114E+00 -8.491889690919E-01
H 1.978825978481E+01 2.820792032177E+00 -9.154305137441E-02
H 1.282788590307E+01 2.740887431479E+00 6.728921956819E-01
H 5.867512021328E+00 2.457703748714E+00 1.387422106862E+00
H -1.470949912409E+00 6.101399162305E-01 3.019252503610E+00
H -8.431323794148E+00 -2.270703037425E-01 3.071904209947E+00
H -1.539169767589E+01 -1.047439758064E+00 2.896726834059E+00
H 1.767007826237E+01 -1.790125397249E+00 2.506712480533E+00
H 1.070970438063E+01 -2.400045624998E+00 1.930786729772E+00
H 3.749330498895E+00 -2.831965448219E+00 1.211663360025E+00
H -3.211043382844E+00 -3.053851349526E+00 4.026764618560E-01
H -1.017141726458E+01 -3.049247066678E+00 -4.361751073663E-01
H -1.713179114632E+01 -2.818494078273E+00 -1.242677564244E+00
H 1.592998479194E+01 -2.378706277834E+00 -1.957016311053E+00
H 8.969610910200E+00 -1.762500714625E+00 -2.526212110825E+00
H 2.009237028461E+00 -1.015578536317E+00 -2.908050314988E+00
H -4.951136853279E+00 -1.933355439333E-01 -3.074211730734E+00
H -1.191151073502E+01 6.432462612930E-01 -3.012372925995E+00

H -1.887188461676E+01 1.432121433975E+00 -2.727120202023E+00
H 1.418989132150E+01 2.114782711419E+00 -2.239609448412E+00
H 7.229517439765E+00 2.640600229644E+00 -1.585997107544E+00
H 2.691435580257E-01 2.970576508778E+00 -8.147586166634E-01
H -6.691230323713E+00 3.080238717740E+00 1.690679354256E-02
H -1.365160420545E+01 2.961453712162E+00 8.473183042149E-01
H 1.941017173281E+01 2.623031232501E+00 1.614888092487E+00
H 1.244979785107E+01 2.090070525896E+00 2.262689018561E+00
H 5.489423969330E+00 1.402098849821E+00 2.742676651241E+00
H 7.803376727655E-02 1.426417218840E+00 3.179809072178E+00
H -6.882340114463E+00 5.156195784222E-01 3.446735886031E+00
H -1.384271399620E+01 -4.334192073246E-01 3.458034066985E+00
H 1.921906194206E+01 -1.350313273225E+00 3.212865680644E+00
H 1.225868806032E+01 -2.167060780923E+00 2.729413744652E+00
H 5.298314178581E+00 -2.823087304143E+00 2.043533677456E+00
H -1.662059703158E+00 -3.269738356779E+00 1.206094065948E+00
H -8.622433584897E+00 -3.473887873551E+00 2.792039750816E-01
H -1.558280746664E+01 -3.420395018722E+00 -6.683933973434E-01
H 1.747896847162E+01 -3.113227112620E+00 -1.566419089184E+00
H 1.051859458989E+01 -2.575165393641E+00 -2.348270643070E+00
H 3.558220708146E+00 -1.846115438013E+00 -2.955961705983E+00
H -3.402153173593E+00 -9.801475457647E-01 -3.344422611788E+00
H -1.036252705533E+01 -4.148659392334E-02 -3.484842992193E+00
H -1.732290093707E+01 9.002512288008E-01 -3.366808509962E+00
H 1.573887500119E+01 1.775221536260E+00 -2.999073242671E+00
H 8.778501119450E+00 2.518531783473E+00 -2.408910432819E+00
H 1.818127237711E+00 3.075054049822E+00 -1.640089756197E+00
H -5.142246644028E+00 3.403513624732E+00 -7.496311252684E-01
H -1.210262052577E+01 3.479550164135E+00 1.964242168868E-01
H -1.906299440751E+01 3.297524385746E+00 1.127911673456E+00
H 1.399878153075E+01 2.870936308837E+00 1.975747081058E+00
H 7.038407649016E+00 2.231424019561E+00 2.677050366100E+00

PbE0/POB-TZVP optimized geometry, *all*-[60.1]-$(GeMe_2)_\infty$

Energy (a.u): -2.8034646223699E+04
Unit cell length (Å): 20.46661067

Ge	1.059959419294E-01	-1.517587180825E-01	1.366474298441E+00
Ge	-6.191422725763E+00	-7.694079418593E-01	1.139427108602E+00
Ge	7.977769276545E+00	-1.210795078527E+00	6.513508997679E-01
Ge	1.680350608852E+00	-1.374803654367E+00	1.405804942606E-02
Ge	-4.617068058840E+00	-1.223861281171E+00	-6.264553306215E-01
Ge	9.552123943468E+00	-7.925470375865E-01	-1.123455344029E+00
Ge	3.254705275776E+00	-1.796698189180E-01	-1.363085277224E+00
Ge	-3.042713391917E+00	4.743675900086E-01	-1.290448800365E+00
Ge	-9.340132059609E+00	1.019733100813E+00	-9.221860549366E-01
Ge	4.829059942699E+00	1.331490047338E+00	-3.426615978689E-01
Ge	-1.468358724994E+00	1.338218670212E+00	3.153625017505E-01
Ge	-7.765777392686E+00	1.038377523024E+00	9.011408527491E-01
Ge	6.403414609622E+00	5.006565991162E-01	1.280478694307E+00
C	-8.662116760039E-01	-1.508711667187E+00	2.406332853877E+00
C	-7.163630343696E+00	-2.454176473531E+00	1.429568653518E+00
C	7.005561658611E+00	-2.837419025822E+00	1.253075028081E-01
C	7.081429909191E-01	-2.570643073903E+00	-1.207660086676E+00
C	-5.589275676773E+00	-1.714963773360E+00	-2.263967304185E+00
C	8.579916325535E+00	-4.664069398945E-01	-2.801626896068E+00
C	2.282497657842E+00	8.889981026879E-01	-2.697467529327E+00
C	-4.014921009850E+00	2.040744393533E+00	-1.975350859624E+00
C	1.015427099246E+01	2.724980737456E+00	-8.007051135402E-01
C	3.856852324765E+00	2.784956834005E+00	5.573725245130E-01
C	-2.440566342927E+00	2.206932882252E+00	1.787762834267E+00
C	-8.737985010619E+00	1.123327203600E+00	2.608598223569E+00
C	5.431206991688E+00	-2.176191998372E-01	2.831835196867E+00
C	1.079107748789E+00	9.417300154280E-01	2.677578667634E+00
C	-5.218310918904E+00	-4.104723351204E-01	2.808521925396E+00
C	8.950881083404E+00	-1.668640420421E+00	2.296066656407E+00
C	2.653462415712E+00	-2.544543094699E+00	1.257610187039E+00
C	-3.643956251981E+00	-2.837521611051E+00	-6.894962033429E-02
C	-9.941374919673E+00	-2.480458122154E+00	-1.379713900622E+00
C	4.227817082635E+00	-1.555151570231E+00	-2.374402353632E+00
C	-2.069601585058E+00	-2.735785351773E-01	-2.825143842075E+00
C	-8.367020252750E+00	1.070668045307E+00	-2.628678922973E+00
C	5.802171749558E+00	2.169637479560E+00	-1.830015341633E+00
C	-4.952469181345E-01	2.771569114212E+00	-6.121172996008E-01
C	-6.792665585827E+00	2.738567665827E+00	7.460094389572E-01
C	7.376526416481E+00	2.078193368519E+00	1.933234405438E+00
H	-1.764196073017E+00	-1.094767141007E+00	2.867883782972E+00

H -8.061614740709E+00 -2.302140210367E+00 2.030621318088E+00
H 6.107577261598E+00 -2.982120701330E+00 7.281679808691E-01
H -1.898414060938E-01 -2.978933278068E+00 -7.410998653911E-01
H -6.487260073786E+00 -2.293308140838E+00 -2.040590663712E+00
H 7.681931928522E+00 -1.082313745902E+00 -2.872606732759E+00
H 1.384513260829E+00 3.766256849262E-01 -3.046543217996E+00
H -4.912905406863E+00 1.749284710169E+00 -2.522553366815E+00
H 9.256286595445E+00 2.721203689478E+00 -1.420676939361E+00
H 2.958867927752E+00 3.069727697588E+00 6.659453887912E-03
H -3.338550739940E+00 2.715014084409E+00 1.432470246506E+00
H -9.635969407632E+00 1.738323463958E+00 2.530119368788E+00
H 4.533222594675E+00 3.634038869838E-01 3.048148634924E+00
H -2.371677430642E-01 -1.897758497506E+00 3.208006348857E+00
H -6.534586410757E+00 -3.171216583229E+00 1.958616203195E+00
H 7.634605591551E+00 -3.718187167036E+00 2.605306892654E-01
H 1.337186923859E+00 -3.413365879889E+00 -1.497239265840E+00
H -4.960231743833E+00 -2.326583605177E+00 -2.912009748831E+00
H 9.208960258474E+00 -7.068090648911E-01 -3.659673891886E+00
H 2.911541590782E+00 1.074886914189E+00 -3.568950850162E+00
H -3.385877076910E+00 2.610339255020E+00 -2.660624179186E+00
H -9.683295744603E+00 3.547794330524E+00 -1.142780572755E+00
H 4.485896257705E+00 3.672492480461E+00 6.368602908942E-01
H -1.811522409987E+00 2.955866861458E+00 2.270604136898E+00
H -8.108941077680E+00 1.562087766551E+00 3.384179938885E+00
H 6.060250924628E+00 -1.895468104739E-01 3.722480900663E+00
H -1.168326168999E+00 -2.356325371611E+00 1.792072613276E+00
H -7.465744836691E+00 -2.919240168067E+00 4.917624927711E-01
H 6.703447165616E+00 -2.813392222676E+00 -9.212044884473E-01
H 4.060284979240E-01 -2.063030024123E+00 -2.123134623080E+00
H -5.891390169768E+00 -8.400525092492E-01 -2.838680202111E+00
H 8.277801832539E+00 5.753709117630E-01 -2.903918356643E+00
H 1.980383164847E+00 1.858983790861E+00 -2.303903811678E+00
H -4.317035502845E+00 2.716725886657E+00 -1.176092668509E+00
H 9.852156499463E+00 2.952098821915E+00 2.211471315628E-01
H 3.554737831770E+00 2.511181493720E+00 1.567724788905E+00
H -2.742680835922E+00 1.494982748332E+00 2.555155590241E+00
H -9.040099503614E+00 1.363014717956E-01 2.957231038816E+00
H 5.129092498693E+00 -1.253604829318E+00 2.681840494896E+00
H 1.524794887103E+00 1.824491208997E+00 2.221037887000E+00
H -4.772623780589E+00 5.833389626817E-01 2.814514722259E+00
H 9.396568221719E+00 -7.914492099874E-01 2.763220153228E+00
H 3.099149554027E+00 -1.984925906645E+00 2.078905147505E+00
H -3.198269113666E+00 -2.723679999041E+00 9.183380260121E-01
H -9.495687781358E+00 -2.838471827559E+00 -4.526092700677E-01
H 4.673504220950E+00 -2.303003967677E+00 -1.719869236908E+00

H -1.623914446743E+00 -1.239945653006E+00 -2.593127888244E+00
H -7.921333114435E+00 1.071692678030E-01 -2.872332190962E+00
H 6.247858887873E+00 1.429733000888E+00 -2.493519804086E+00
H -4.955977981959E-02 2.424762133620E+00 -1.543472080265E+00
H -6.346978447512E+00 2.864307483092E+00 -2.398335037104E-01
H 7.822213554796E+00 2.647674506834E+00 1.118748038237E+00
H 4.091447812433E-01 1.286082389765E+00 3.466309123374E+00
H -5.888273886449E+00 -4.721047695947E-01 3.666936587749E+00
H 8.280918115859E+00 -2.122138415720E+00 3.027513071248E+00
H 1.983499448166E+00 -3.286015725343E+00 1.694522795611E+00
H -4.313919219526E+00 -3.697106433073E+00 -2.666223128660E-02
H 9.855272782782E+00 -3.261234611949E+00 -1.741739262311E+00
H 3.557854115089E+00 -2.078253243364E+00 -3.057804818574E+00
H -2.739564552603E+00 -4.191691023918E-01 -3.673364141444E+00
H -9.036983220295E+00 1.335941628403E+00 -3.447400008347E+00
H 5.132208782013E+00 2.785004231973E+00 -2.431678079010E+00
H -1.165209885680E+00 3.596055928938E+00 -8.588880066707E-01
H -7.462628553372E+00 3.583294549754E+00 9.106629572748E-01
H 6.706563448936E+00 2.749643572603E+00 2.471592012387E+00
H 1.878789003509E+00 3.711912560570E-01 3.152646487084E+00
H -4.418629664183E+00 -1.136434341465E+00 2.964031006693E+00
H 9.750562338124E+00 -2.383716526876E+00 2.096391743114E+00
H 3.453143670432E+00 -3.084917982877E+00 7.484943954471E-01
H -2.844274997260E+00 -3.079401906294E+00 -7.708739978814E-01
H -9.141693664953E+00 -2.368431963794E+00 -2.113644448334E+00
H 5.027498337355E+00 -1.114882801089E+00 -2.972204427850E+00
H -1.269920330337E+00 3.940725755517E-01 -3.149868191892E+00
H -7.567338998030E+00 1.812750674223E+00 -2.605935113198E+00
H 6.601853004278E+00 2.816149439443E+00 -1.465013704994E+00
H 3.044343365858E-01 3.174402306367E+00 1.152468769632E-02
H -5.992984331106E+00 2.805437860597E+00 1.485422913323E+00
H 8.176207671201E+00 1.793781410156E+00 2.619028650793E+00

PbE0/POB-TZVP optimized geometry, *all*-[-52.5]-$(GeMe_2)_\infty$

Energy (a.u): -3.0191154811786E+04
Unit cell length (Å): 20.85316212

Ge	1.736095454591E-01	-1.577972485681E-01	1.510564059544E+00
Ge	-7.273948354541E+00	-7.975795907321E-01	1.292505530390E+00
Ge	6.131655865459E+00	-1.279391513280E+00	8.184504294026E-01
Ge	-1.315902034541E+00	-1.507804255915E+00	1.822911832360E-01
Ge	-8.763459934541E+00	-1.437577873661E+00	-4.899730674251E-01
Ge	4.642144285459E+00	-1.082621562793E+00	-1.065192142957E+00
Ge	-2.805413614541E+00	-5.132387739310E-01	-1.429436850853E+00
Ge	-1.025297151454E+01	1.577972485681E-01	-1.510564059544E+00
Ge	3.152632705459E+00	7.975795907321E-01	-1.292505530390E+00
Ge	-4.294925194541E+00	1.279391513280E+00	-8.184504294026E-01
Ge	9.110679025459E+00	1.507804255915E+00	-1.822911832360E-01
Ge	1.663121125459E+00	1.437577873661E+00	4.899730674251E-01
Ge	-5.784436774541E+00	1.082621562793E+00	1.065192142957E+00
Ge	7.621167445459E+00	5.132387739310E-01	1.429436850853E+00
C	1.242262696346E+00	-1.424551451141E+00	2.567261402105E+00
C	-6.205295203654E+00	-2.397369484641E+00	1.694932888878E+00
C	7.200309016346E+00	-2.895359089900E+00	4.869021300205E-01
C	-2.472488836543E-01	-2.819887318156E+00	-8.175655671501E-01
C	-7.694806783654E+00	-2.185902279402E+00	-1.960104376963E+00
C	5.710797436346E+00	-1.118972485881E+00	-2.714420475816E+00
C	-1.736760463654E+00	1.695835317658E-01	-2.931112309251E+00
C	-9.184318363654E+00	1.424551451141E+00	-2.567261402105E+00
C	4.221285856346E+00	2.397369484641E+00	-1.694932888878E+00
C	-3.226272043654E+00	2.895359089900E+00	-4.869021300205E-01
C	1.017933217635E+01	2.819887318156E+00	8.175655671501E-01
C	2.731774276346E+00	2.185902279402E+00	1.960104376963E+00
C	-4.715783623654E+00	1.118972485881E+00	2.714420475816E+00
C	8.689820596346E+00	-1.695835317658E-01	2.931112309251E+00
C	-8.947215193207E-01	8.630337793809E-01	2.806657814525E+00
C	-8.342279419321E+00	-4.401966198193E-01	2.903167636925E+00
C	5.063324800679E+00	-1.656240679807E+00	2.424669503817E+00
C	-2.384233099321E+00	-2.544245960700E+00	1.465935838858E+00
C	-9.831790999321E+00	-2.928332125947E+00	2.168556024903E-01
C	3.573813220679E+00	-2.732426200014E+00	-1.075175545510E+00
C	-3.873744679321E+00	-1.995329754160E+00	-2.154254990560E+00
C	9.531859540679E+00	-8.630337793809E-01	-2.806657814525E+00
C	2.084301640679E+00	4.401966198193E-01	-2.903167636925E+00
C	-5.363256259321E+00	1.656240679807E+00	-2.424669503817E+00
C	8.042347960679E+00	2.544245960700E+00	-1.465935838858E+00
C	5.947900606793E-01	2.928332125947E+00	-2.168556024903E-01

C -6.852767839321E+00 2.732426200014E+00 1.075175545510E+00
C 6.552836380679E+00 1.995329754160E+00 2.154254990560E+00
H 6.039569343273E-01 -2.127535529129E+00 3.104286370745E+00
H -6.843600965673E+00 -3.263742654932E+00 1.873762306611E+00
H 6.562003254327E+00 -3.753525520749E+00 2.721166374662E-01
H -8.855546456727E-01 -3.499876623212E+00 -1.383425069020E+00
H -8.333112545673E+00 -2.553034237278E+00 -2.764962473992E+00
H 5.072491674327E+00 -1.100532109741E+00 -3.598865150951E+00
H -2.375066225673E+00 5.699438992710E-01 -3.719968447579E+00
H -9.822624125673E+00 2.127535529129E+00 -3.104286370745E+00
H 3.582980094327E+00 3.263742654932E+00 -1.873762306611E+00
H -3.864577805673E+00 3.753525520749E+00 -2.721166374662E-01
H 9.541026414327E+00 3.499876623212E+00 1.383425069020E+00
H 2.093468514327E+00 2.553034237278E+00 2.764962473992E+00
H -5.354089385673E+00 1.100532109741E+00 3.598865150951E+00
H 8.051514834327E+00 -5.699438992710E-01 3.719968447579E+00
H 1.846223393118E+00 -8.995374855014E-01 3.308510282715E+00
H -5.601334506882E+00 -2.245964082321E+00 2.590570076175E+00
H 7.804269713118E+00 -3.147549947696E+00 1.359535694792E+00
H 3.567118131180E-01 -3.425724943762E+00 -1.407714045554E-01
H -7.090846086882E+00 -3.025393100957E+00 -1.613197000783E+00
H 6.314758133118E+00 -2.025845050496E+00 -2.766109146443E+00
H -1.132799766882E+00 -6.250535424253E-01 -3.371159451547E+00
H -8.580357666882E+00 8.995374855014E-01 -3.308510282715E+00
H 4.825246553118E+00 2.245964082321E+00 -2.590570076175E+00
H -2.622311346882E+00 3.147549947696E+00 -1.359535694792E+00
H -1.006986924688E+01 3.425724943762E+00 1.407714045554E-01
H 3.335734973118E+00 3.025393100957E+00 1.613197000783E+00
H -4.111822926882E+00 2.025845050496E+00 2.766109146443E+00
H 9.293781293118E+00 6.250535424253E-01 3.371159451547E+00
H 1.920987127308E+00 -2.009123941334E+00 1.947006028280E+00
H -5.526570772692E+00 -2.654932378534E+00 8.824656090820E-01
H 7.879033447308E+00 -2.774898897556E+00 -3.568579467251E-01
H 4.314755473081E-01 -2.345262658016E+00 -1.525501409608E+00
H -7.016082352692E+00 -1.451118386297E+00 -2.392000609271E+00
H 6.389521867308E+00 -2.695623213724E-01 -2.784734752305E+00
H -1.058036032692E+00 9.653838672648E-01 -2.625918025115E+00
H -8.505593932692E+00 2.009123941334E+00 -1.947006028280E+00
H 4.900010287308E+00 2.654932378534E+00 -8.824656090820E-01
H -2.547547612692E+00 2.774898897556E+00 3.568579467251E-01
H -9.995105512692E+00 2.345262658016E+00 1.525501409608E+00
H 3.410498707308E+00 1.451118386297E+00 2.392000609271E+00
H -4.037059192692E+00 2.695623213724E-01 2.784734752305E+00
H 9.368545027308E+00 -9.653838672648E-01 2.625918025115E+00
H -1.573414216272E+00 1.563410426129E+00 2.320905951913E+00

H -9.020972116272E+00 4.015807691401E-01 2.769402369467E+00
H 4.384632103728E+00 -8.397868842420E-01 2.669384683257E+00
H -3.062925796272E+00 -1.914824445890E+00 2.040662622674E+00
H 1.034267842373E+01 -2.610607542248E+00 1.007762302585E+00
H 2.895120523728E+00 -2.789327797864E+00 -2.247377009246E-01
H -4.552437376272E+00 -2.415587474252E+00 -1.412725646539E+00
H 8.853166843728E+00 -1.563410426129E+00 -2.320905951913E+00
H 1.405608943728E+00 -4.015807691401E-01 -2.769402369467E+00
H -6.041948956272E+00 8.397868842420E-01 -2.669384683257E+00
H 7.363655263728E+00 1.914824445890E+00 -2.040662622674E+00
H -8.390263627233E-02 2.610607542248E+00 -1.007762302585E+00
H -7.531460536272E+00 2.789327797864E+00 2.247377009246E-01
H 5.874143683728E+00 2.415587474252E+00 1.412725646539E+00
H -1.498688902196E+00 1.961162905776E-01 3.423323610903E+00
H -8.946246802196E+00 -1.308629776209E+00 3.169399667637E+00
H 4.459357417804E+00 -2.554185666527E+00 2.287737250059E+00
H -2.988200482196E+00 -3.293853760557E+00 9.529604128505E-01
H 1.041740373780E+01 -3.381133720844E+00 -5.705619214152E-01
H 2.969845837804E+00 -2.798738680834E+00 -1.981077469662E+00
H -4.477712062196E+00 -1.662019120807E+00 -2.999216328721E+00
H 8.927892157804E+00 -1.961162905776E-01 -3.423323610903E+00
H 1.480334257803E+00 1.308629776209E+00 -3.169399667637E+00
H -5.967223642196E+00 2.554185666527E+00 -2.287737250059E+00
H 7.438380577803E+00 3.293853760557E+00 -9.529604128505E-01
H -9.177322196496E-03 3.381133720844E+00 5.705619214152E-01
H -7.456735222196E+00 2.798738680834E+00 1.981077469662E+00
H 5.948868997804E+00 1.662019120807E+00 2.999216328721E+00
H -2.562278997686E-01 1.439572113825E+00 3.477425194576E+00
H -7.703785799769E+00 -2.117885882674E-01 3.757658772248E+00
H 5.701818420231E+00 -1.821201963037E+00 3.293641945416E+00
H -1.745739479769E+00 -3.069903953451E+00 2.177278937427E+00
H -9.193297379769E+00 -3.710573815982E+00 6.296791333063E-01
H 4.212306840231E+00 -3.616319027057E+00 -1.042636345673E+00
H -3.235251059769E+00 -2.805807903581E+00 -2.508444909297E+00
H 1.017035316023E+01 -1.439572113825E+00 -3.477425194576E+00
H 2.722795260231E+00 2.117885882674E-01 -3.757658772248E+00
H -4.724762639769E+00 1.821201963037E+00 -3.293641945416E+00
H 8.680841580231E+00 3.069903953451E+00 -2.177278937427E+00
H 1.233283680231E+00 3.710573815982E+00 -6.296791333063E-01
H -6.214274219769E+00 3.616319027057E+00 1.042636345673E+00
H 7.191330000231E+00 2.805807903581E+00 2.508444909297E+00

PbE0/POB-TZVP optimized geometry, *all*-[-35.5]-$(GeMe_2)_\infty$

Energy (a.u): -4.9599720833059E+04
Unit cell length (Å): 29.17310618

Ge	-3.097458362546E-05	-6.809737578093E-02	1.968620042494E+00
Ge	-7.610406499801E+00	-5.966994714624E-01	1.877245819027E+00
Ge	1.395232415498E+01	-1.081047097064E+00	1.646644860991E+00
Ge	6.341948629764E+00	-1.485218404938E+00	1.293919786514E+00
Ge	-1.268426895453E+00	-1.779237858139E+00	8.452306007604E-01
Ge	-8.878802420671E+00	-1.941299378874E+00	3.338545280213E-01
Ge	1.268392823411E+01	-1.959383605532E+00	-2.022820077783E-01
Ge	5.073552708895E+00	-1.832149313751E+00	-7.234162124396E-01
Ge	-2.536822816323E+00	-1.569032888894E+00	-1.190897946033E+00
Ge	-1.014719834154E+01	-1.189548472516E+00	-1.570056226965E+00
Ge	1.141553231324E+01	-7.218406877536E-01	-1.832770620072E+00
Ge	3.805156788025E+00	-2.005972813820E-01	-1.959556800657E+00
Ge	-3.805218737192E+00	3.355235076782E-01	-1.941011617712E+00
Ge	-1.141559426241E+01	8.467600530919E-01	-1.778510482619E+00
Ge	1.014713639237E+01	1.295196279037E+00	-1.484105361174E+00
Ge	2.536760867155E+00	1.647573722095E+00	-1.079630934421E+00
Ge	-5.073614658062E+00	1.877758159333E+00	-5.950852202452E-01
Ge	-1.268399018328E+01	1.968677864066E+00	-6.640475761739E-02
Ge	8.878740471503E+00	1.913589737723E+00	4.672006421014E-01
Ge	1.268364946286E+00	1.716579414623E+00	9.661559074962E-01
Ge	-6.342010578932E+00	1.392258249169E+00	1.393455809101E+00
Ge	-1.395238610415E+01	9.646796585320E-01	1.717409467981E+00
Ge	7.610344550634E+00	4.655551907374E-01	1.913990723247E+00
C	1.228402066570E+00	-1.077226902297E+00	3.126454869305E+00
C	-6.381973458648E+00	-1.880787835525E+00	2.719885101723E+00
C	-1.399234898387E+01	-2.544859339023E+00	2.111593898793E+00
C	7.570381670917E+00	-3.020190267303E+00	1.346695436289E+00
C	-3.999385429998E-02	-3.271527499908E+00	4.819187339967E-01
C	-7.650369379517E+00	-3.280230504088E+00	-4.185996761645E-01
C	1.391236127527E+01	-3.045653817835E+00	-1.288072463311E+00
C	6.301985750048E+00	-2.585194920853E+00	-2.062014808393E+00
C	-1.308389775170E+00	-1.933003943071E+00	-2.683026948226E+00
C	-8.918765300387E+00	-1.137450905736E+00	-3.105051253341E+00
C	1.264396535440E+01	-2.575383382137E-01	-3.296788111660E+00
C	5.033589829178E+00	6.414746696940E-01	-3.244017277539E+00
C	-2.576785696039E+00	1.492912435902E+00	-2.950652522335E+00
C	-1.018716122126E+01	2.233627716359E+00	-2.438451367886E+00
C	1.137556943353E+01	2.808685047260E+00	-1.745401430654E+00
C	3.765193908309E+00	3.175435057086E+00	-9.229030539909E-01
C	-3.845181616909E+00	3.306677575376E+00	-3.195717981338E-02

C -1.145555714213E+01 3.192678944943E+00 8.613588121965E-01
C 1.010717351266E+01 2.841893922699E+00 1.690791761560E+00
C 2.496797987439E+00 2.280338629008E+00 2.394826420826E+00
C -5.113577537778E+00 1.549661051058E+00 2.921247760062E+00
C -1.272395306300E+01 7.040522021789E-01 3.231013516753E+00
C 8.838777591787E+00 -1.937729777113E-01 3.301149781810E+00
C -1.228394254173E+00 8.584899687596E-01 3.193576067065E+00
C -8.838769779390E+00 -3.496167940519E-02 3.306767425079E+00
C 1.272396087539E+01 -9.258203797475E-01 3.174710970630E+00
C 5.113585350175E+00 -1.748015217870E+00 2.807200726825E+00
C -2.496790175042E+00 -2.440567763921E+00 2.231493247200E+00
C -1.010716570026E+01 -2.952114563777E+00 1.490286121833E+00
C 1.145556495452E+01 -3.244716531463E+00 6.385512924146E-01
C 3.845189429306E+00 -3.296672717600E+00 -2.605419651841E-01
C -3.765186095912E+00 -3.104129769547E+00 -1.140312017125E+00
C -1.137556162113E+01 -2.681367716936E+00 -1.935510343337E+00
C 1.018716903365E+01 -2.059740887201E+00 -2.587160721753E+00
C 2.576793508436E+00 -1.285352498550E+00 -3.046933224911E+00
C -5.033582016781E+00 -4.156353951771E-01 -3.280728629568E+00
C -1.264395754200E+01 4.849074840502E-01 -3.271207400105E+00
C 8.918773112784E+00 1.349486993490E+00 -3.019075682555E+00
C 1.308397587566E+00 2.113981226114E+00 -2.543032932981E+00
C -6.301977937651E+00 2.721691142018E+00 -1.878385064370E+00
C -1.391235346287E+01 3.127545676828E+00 -1.074425968575E+00
C 7.650377191914E+00 3.301444456356E+00 -1.907816138621E-01
C 4.000166669676E-02 3.230490203660E+00 7.070121403832E-01
C -7.570373858521E+00 2.919945271068E+00 1.552370038542E+00
C 1.399235679626E+01 2.392841355581E+00 2.282595752562E+00
C 6.381981271045E+00 1.688271343272E+00 2.843531781795E+00
H 1.986028091415E+00 -1.614683119748E+00 2.556886939554E+00
H -5.624347433803E+00 -2.244646130099E+00 2.026434343741E+00
H -1.323472295902E+01 -2.708134005554E+00 1.345690382972E+00
H 8.328007695763E+00 -2.970771970705E+00 5.651427226227E-01
H 7.176321705452E-01 -3.013081369167E+00 -2.573189881079E-01
H -6.892743354672E+00 -2.831924306407E+00 -1.060696526647E+00
H -1.450311887989E+01 -2.440736373033E+00 -1.785407056167E+00
H 7.059611774893E+00 -1.868530188497E+00 -2.377702112026E+00
H -5.507637503244E-01 -1.157743667838E+00 -2.793653879500E+00
H -8.161139275542E+00 -3.610925956589E-01 -3.002413118846E+00
H 1.340159137924E+01 4.623390624510E-01 -2.988497112295E+00
H 5.791215854023E+00 1.251481147359E+00 -2.752937946388E+00
H -1.819159671194E+00 1.947806600713E+00 -2.313205966852E+00
H -9.429535196411E+00 2.499672149115E+00 -1.701914082967E+00
H 1.213319545837E+01 2.866148449456E+00 -9.643990172870E-01
H 4.522819933154E+00 3.020055631057E+00 -1.553588883270E-01

H -3.087555592064E+00 2.949979102338E+00 6.652034986605E-01
H -1.069793111728E+01 2.661116118855E+00 1.436430785256E+00
H 1.086479953750E+01 2.174890326633E+00 2.101124571743E+00
H 3.254424012284E+00 1.527362868345E+00 2.609987560748E+00
H -4.355951512933E+00 7.665578933330E-01 2.925279712272E+00
H -1.196632703815E+01 -5.109917385887E-02 3.023617249801E+00
H 9.596403616632E+00 -8.649664490888E-01 2.897706928040E+00
H 6.903785045869E-01 -1.812266730335E+00 3.727122551958E+00
H -6.919997020630E+00 -2.750628594150E+00 3.099967025025E+00
H -1.453037254585E+01 -3.484988918425E+00 2.242901125250E+00
H 7.032358108935E+00 -3.960883557384E+00 1.219489509607E+00
H -5.780174162826E-01 -4.143017582728E+00 1.056339358283E-01
H -8.188392941500E+00 -4.017882947006E+00 -1.016056023727E+00
H 1.337433771328E+01 -3.594760313696E+00 -2.062389756150E+00
H 5.763962188065E+00 -2.905030752853E+00 -2.955765475164E+00
H -1.846413337152E+00 -1.999848350702E+00 -3.629925590613E+00
H -9.456788862370E+00 -9.463463450776E-01 -4.034870730811E+00
H 1.210594179241E+01 1.773418397150E-01 -4.140567967209E+00
H 4.495566267196E+00 1.287877391541E+00 -3.939178219318E+00
H -3.114809258022E+00 2.302896968883E+00 -3.445637643442E+00
H -1.072518478324E+01 3.147121213096E+00 -2.696549886294E+00
H 1.083754587154E+01 3.757937874055E+00 -1.747471359975E+00
H 3.227170346326E+00 4.090045474318E+00 -6.687908770366E-01
H -4.383205178891E+00 4.118813112463E+00 4.594907657373E-01
H -1.199358070411E+01 3.842107224373E+00 1.553694080447E+00
H 9.569149950674E+00 3.280449819922E+00 2.532667012887E+00
H 1.958774425456E+00 2.475496459387E+00 3.323803619162E+00
H -5.651601099761E+00 1.486946851102E+00 3.868428916394E+00
H -1.326197662498E+01 3.881171972002E-01 4.126150537781E+00
H 8.300754029804E+00 -7.394973337000E-01 4.077854449664E+00
H 1.746529553027E+00 -4.082660223371E-01 3.814984163872E+00
H -5.863845972190E+00 -1.422396820173E+00 3.563365347751E+00
H -1.347422149741E+01 -2.331034952889E+00 3.047468025099E+00
H 8.088509157375E+00 -3.066790886925E+00 2.305553940263E+00
H 4.781336321579E-01 -3.575096970512E+00 1.392647466886E+00
H -7.132241893060E+00 -3.818254466777E+00 3.764547018287E-01
H 1.443048876172E+01 -3.778229496592E+00 -6.676579862980E-01
H 6.820113236506E+00 -3.457990528896E+00 -1.662253535913E+00
H -7.902622887117E-01 -2.881288222925E+00 -2.533567345073E+00
H -8.400637813929E+00 -2.090893950477E+00 -3.216978054549E+00
H 1.316209284085E+01 -1.145427638924E+00 -3.661800218414E+00
H 5.551717315636E+00 -1.150101993762E-01 -3.835043411701E+00
H -2.058658209581E+00 9.239370205232E-01 -3.723858979298E+00
H -9.669033734799E+00 1.894360058341E+00 -3.336492961921E+00
H 1.189369691998E+01 2.724287076752E+00 -2.701674524999E+00

H 4.283321394767E+00 3.352166185465E+00 -1.866485247896E+00
H -3.327054130451E+00 3.731430463342E+00 -8.928672985588E-01
H -1.093742965567E+01 3.833951613911E+00 1.469705337167E-01
H 1.062530099911E+01 3.652126112438E+00 1.175908233852E+00
H 3.014925473897E+00 3.199439124570E+00 2.117634199705E+00
H -4.595450051320E+00 2.509464373294E+00 2.902304924497E+00
H -1.220582557654E+01 1.633374129485E+00 3.471724970201E+00
H 9.356905078245E+00 6.361439986827E-01 3.783663056950E+00
H -1.746597306887E+00 1.434303693986E-01 3.834041748035E+00
H -9.356972832104E+00 -8.963005018765E-01 3.730562130146E+00
H 1.220575782268E+01 -1.869556865229E+00 3.350403785250E+00
H 4.595382297461E+00 -2.704156748542E+00 2.721761318679E+00
H -3.014993227756E+00 -3.338201696509E+00 1.891258266332E+00
H -1.062536875297E+01 -3.724667495902E+00 9.204892403011E-01
H 1.093736190181E+01 -3.834891746345E+00 -1.185482617244E-01
H 3.326986376592E+00 -3.660699619423E+00 -1.148793581500E+00
H -4.283389148626E+00 -3.215010148316E+00 -2.093838136717E+00
H -1.189376467384E+01 -2.530878082200E+00 -2.883592296005E+00
H 9.668965980940E+00 -1.659042366725E+00 -3.459483606256E+00
H 2.058590455722E+00 -6.641630685230E-01 -3.778800843515E+00
H -5.551785069495E+00 3.799741661270E-01 -3.817861709074E+00
H -1.316216059471E+01 1.395930455142E+00 -3.573769237227E+00
H 8.400570060070E+00 2.308356968255E+00 -3.064626649961E+00
H 7.901945348526E-01 3.049583205064E+00 -2.328194723801E+00
H -6.820180990365E+00 3.564635806468E+00 -1.419091245759E+00
H -1.443055651558E+01 3.815315677230E+00 -4.047402619293E-01
H 7.132174139200E+00 3.783031038119E+00 6.396284555640E-01
H -4.782013860170E-01 3.470176293127E+00 1.636558856614E+00
H -8.088576911234E+00 2.899954447474E+00 2.512113174027E+00
H 1.347415374355E+01 2.114656246860E+00 3.201355549475E+00
H 5.863778218331E+00 1.172523666326E+00 3.653168029046E+00
H -1.985974187801E+00 1.434174068773E+00 2.662609149868E+00
H -9.596349713018E+00 6.626276523999E-01 2.950807912890E+00
H 1.196638094176E+01 -1.580628256319E-01 3.020158752062E+00
H 4.356005416547E+00 -9.670305069758E-01 2.865518232900E+00
H -3.254370108670E+00 -1.704277959488E+00 2.498355335277E+00
H -1.086474563389E+01 -2.315126912297E+00 1.945900851652E+00
H 1.069798502090E+01 -2.754273493022E+00 1.249127803764E+00
H 3.087609495678E+00 -2.989148208733E+00 4.597126610502E-01
H -4.522766029540E+00 -3.002331476245E+00 -3.637972666880E-01
H -1.213314155476E+01 -2.792845552917E+00 -1.160326015418E+00
H 9.429589100025E+00 -2.376227051347E+00 -1.870798691722E+00
H 1.819213574808E+00 -1.783374659894E+00 -2.442522787396E+00
H -5.791161950409E+00 -1.058257528313E+00 -2.833096141728E+00
H -1.340153747563E+01 -2.546542770627E-01 -3.013551715779E+00

H 8.161193179156E+00 5.678355169512E-01 -2.970505945153E+00
H 5.508176539385E-01 1.348211548347E+00 -2.707151337736E+00
H -7.059557871279E+00 2.028596896860E+00 -2.243019699992E+00
H 1.450317278350E+01 2.558530493746E+00 -1.612533552232E+00
H 6.892797258286E+00 2.898709588409E+00 -8.624531677527E-01
H -7.175782669310E-01 3.023904653614E+00 -4.840857728221E-02
H -8.327953792149E+00 2.924830544103E+00 7.692262559108E-01
H 1.323477686263E+01 2.608835133346E+00 1.529811096679E+00
H 5.624401337417E+00 2.099354355375E+00 2.176936846826E+00
H -6.903414921545E-01 1.550090704435E+00 3.843764034724E+00
H -8.300717017372E+00 4.555740105996E-01 4.119436304579E+00
H 1.326201363741E+01 -6.727305234896E-01 4.089588828890E+00
H 5.651638112193E+00 -1.751141712189E+00 3.756435258386E+00
H -1.958737413024E+00 -2.699678731036E+00 3.144684069316E+00
H -9.569112938242E+00 -3.447992928610E+00 2.299706048797E+00
H 1.199361771654E+01 -3.940585264187E+00 1.284169351093E+00
H 4.383242191324E+00 -4.140922417697E+00 1.733916873036E-01
H -3.227133333894E+00 -4.034146298947E+00 -9.502456447194E-01
H -1.083750885911E+01 -3.628176004195E+00 -2.003407604358E+00
H 1.072522179567E+01 -2.953120493012E+00 -2.907985986962E+00
H 3.114846270454E+00 -2.059045544490E+00 -3.596892352063E+00
H -4.495529254763E+00 -1.012260607440E+00 -4.019033666099E+00
H -1.210590477998E+01 1.095990680795E-01 -4.143101638976E+00
H 9.456825874802E+00 1.223330282102E+00 -3.959894716720E+00
H 1.846450349585E+00 2.246332685465E+00 -3.483000518637E+00
H -5.763925175633E+00 3.102734869835E+00 -2.747788105754E+00
H -1.337430070085E+01 3.729021402977E+00 -1.808784819361E+00
H 8.188429953932E+00 4.078743477798E+00 -7.356322375565E-01
H 5.780544287150E-01 4.125963807881E+00 3.920788220142E-01
H -7.032321096502E+00 3.867180277361E+00 1.490711188997E+00
H 1.453040955828E+01 3.321585676842E+00 2.478784326643E+00
H 6.920034033063E+00 2.529644261916E+00 3.283017370464E+00

PbE0/POB-TZVP optimized geometry, *all*-[180]-$(SnMe_2)_\infty$

Energy (a.u): -1.6633989312861E+02
Unit cell length (Å): 4.67816633

Sn	-2.936623213741E-01	-2.784959087338E-01	-7.362963042871E-01
Sn	2.045420843626E+00	2.784959087338E-01	7.362963042871E-01
C	-2.936961905320E-01	-2.358717898538E+00	-1.326212344487E+00
C	2.045386974468E+00	2.358717898538E+00	1.326212344487E+00
C	-2.936706900604E-01	8.906494832293E-01	-2.555209941768E+00
C	2.045412474940E+00	-8.906494832293E-01	2.555209941768E+00
H	5.887738413651E-01	-2.586475936185E+00	-1.922243074955E+00
H	-1.750309323635E+00	2.586475936185E+00	1.922243074955E+00
H	-1.176230806763E+00	-2.586463851102E+00	-1.922151919909E+00
H	1.162852358237E+00	2.586463851102E+00	1.922151919909E+00
H	-2.936565025019E-01	-3.009990343823E+00	-4.544899878638E-01
H	2.045426662498E+00	3.009990343823E+00	4.544899878638E-01
H	5.889378583575E-01	6.671003460118E-01	-3.152623178396E+00
H	-1.750145306642E+00	-6.671003460118E-01	3.152623178396E+00
H	-2.938958067948E-01	1.955778375443E+00	-2.332661042207E+00
H	2.045187358205E+00	-1.955778375443E+00	2.332661042207E+00
H	-1.176063358146E+00	6.667653792982E-01	-3.152817490732E+00
H	1.163019806854E+00	-6.667653792982E-01	3.152817490732E+00

PbE0/POB-TZVP optimized geometry, *all*-[165.5]-$(SnMe_2)_\infty$

Energy (a.u): -1.2475503407635E+03
Unit cell length (Å): 34.84347681

Sn	-2.169323446627E-01	6.703032599469E-01	4.379337700663E-01
Sn	-4.862729252663E+00	4.342287868412E-01	6.727093041859E-01
Sn	-9.508526160663E+00	1.230722116460E-01	7.911672882397E-01
Sn	-1.415432306866E+01	-2.093646670187E-01	7.728252606276E-01
Sn	1.604335683334E+01	-5.056004927377E-01	6.208547245559E-01
Sn	1.139755992534E+01	-7.144134000260E-01	3.615327663204E-01
Sn	6.751763017337E+00	-7.996977402078E-01	3.969850836603E-02
Sn	2.105966109337E+00	-7.467070760818E-01	-2.889999823344E-01
Sn	-2.539830798663E+00	-5.646039748804E-01	-5.677277506069E-01
Sn	-7.185627706663E+00	-2.848757171562E-01	-7.482902331547E-01
Sn	-1.183142461466E+01	4.411014007906E-02	-7.994665363867E-01
Sn	-1.647722152266E+01	3.654689533666E-01	-7.124078125520E-01
Sn	1.372045837934E+01	6.236348644358E-01	-5.021673059052E-01
Sn	9.074661471337E+00	7.739686418992E-01	-2.050975100207E-01
Sn	4.428864563337E+00	7.904762098938E-01	1.274355085988E-01
C	-8.763022834285E-02	2.696589137025E+00	-3.054705721844E-01
C	-4.733427136343E+00	2.587702832346E+00	8.177403596857E-01
C	-9.379224044343E+00	2.031379199413E+00	1.799556554428E+00
C	-1.402502095234E+01	1.123811648400E+00	2.470213072452E+00
C	1.617265894966E+01	2.192685387059E-02	2.713747309068E+00
C	1.152686204166E+01	-1.083749292892E+00	2.488049982325E+00
C	6.881065133657E+00	-2.002035341361E+00	1.832146210414E+00
C	2.235268225657E+00	-2.574151291388E+00	8.594477141966E-01
C	-2.410528682343E+00	-2.701173097704E+00	-2.618570996427E-01
C	-7.056325590343E+00	-2.361137536039E+00	-1.337884442057E+00
C	-1.170212249834E+01	-1.612839844133E+00	-2.182579410141E+00
C	-1.634791940634E+01	-5.856674909855E-01	-2.649886570100E+00
C	1.384976049566E+01	5.427720919752E-01	-2.659004268625E+00
C	9.203963587657E+00	1.577361449304E+00	-2.208355972809E+00
C	4.558166679657E+00	2.339210682169E+00	-1.375862867011E+00
C	-3.460011715337E-01	8.034701152982E-01	2.592179999285E+00
C	-4.991798079534E+00	-3.203281169752E-01	2.694875001247E+00
C	-9.637594987534E+00	-1.388738707734E+00	2.331601633322E+00
C	-1.428339189553E+01	-2.217023759630E+00	1.565173161061E+00
C	1.591428800647E+01	-2.661965262458E+00	5.281120300997E-01
C	1.126849109847E+01	-2.646628788212E+00	-6.002644686126E-01
C	6.622694190466E+00	-2.173666152616E+00	-1.624849787470E+00
C	1.976897282466E+00	-1.324856892096E+00	-2.368483816778E+00
C	-2.668899625534E+00	-2.469678389849E-01	-2.702585477164E+00
C	-7.314696533534E+00	8.736241971186E-01	-2.569385556330E+00

C -1.196049344153E+01 1.843158672914E+00 -1.991915530672E+00
C -1.660629034953E+01 2.493994269591E+00 -1.070025213777E+00
C 1.359138955247E+01 2.713595599830E+00 3.688218345513E-02
C 8.945592644466E+00 2.463991598615E+00 1.137412316103E+00
C 4.299795736466E+00 1.788341065340E+00 2.041273526231E+00
H -9.797441866617E-01 3.259820901823E+00 -3.593459187370E-02
H -5.625541094662E+00 2.992610492858E+00 1.293060727457E+00
H -1.027133800266E+01 2.207950542665E+00 2.398474099923E+00
H -1.491713491066E+01 1.041515885044E+00 3.089169511059E+00
H 1.528054499134E+01 -3.050063309758E-01 3.245719449509E+00
H 1.063474808334E+01 -1.598790181474E+00 2.841055008703E+00
H 5.988951175338E+00 -2.616128685043E+00 1.945146346718E+00
H 1.343154267338E+00 -3.181114772185E+00 7.129042102857E-01
H -3.302642640662E+00 -3.196057215695E+00 -6.426055406365E-01
H -7.948439548662E+00 -2.658372331344E+00 -1.887002955695E+00
H -1.259423645666E+01 -1.661030720349E+00 -2.805120416829E+00
H -1.724003336466E+01 -3.764818078149E-01 -3.238207074175E+00
H 1.295764653734E+01 9.731642295201E-01 -3.111378310209E+00
H 8.311849629338E+00 2.154541330652E+00 -2.446563970423E+00
H 3.666052721338E+00 2.963378662320E+00 -1.358716493814E+00
H 8.924972697478E-03 2.708483615633E+00 -1.389349645735E+00
H -4.636871935303E+00 3.039422315126E+00 -1.675945242902E-01
H -9.282668843303E+00 2.844817284048E+00 1.083139212953E+00
H -1.392846575130E+01 2.158317500205E+00 2.146588340265E+00
H 1.626921415070E+01 1.098625012878E+00 2.838872842403E+00
H 1.162341724270E+01 -1.510297198711E-01 3.040290439740E+00
H 6.977620334698E+00 -1.374570041992E+00 2.716014199873E+00
H 2.331823426697E+00 -2.360434716276E+00 1.922114430635E+00
H -2.313973481302E+00 -2.938158784240E+00 7.958636144776E-01
H -6.959770389302E+00 -3.007848506074E+00 -4.679992508164E-01
H -1.160556729730E+01 -2.557453895762E+00 -1.650940794005E+00
H -1.625136420530E+01 -1.664852273133E+00 -2.548419675583E+00
H 1.394631569670E+01 -4.843825677719E-01 -3.005253643587E+00
H 9.300518788698E+00 7.798412840347E-01 -2.942451954743E+00
H 4.654721880697E+00 1.909223493196E+00 -2.370873591587E+00
H -4.441098730863E-01 -1.842408381283E-01 3.038350324396E+00
H -5.089906781086E+00 -1.404120792217E+00 2.700733637561E+00
H -9.735703689086E+00 -2.381215505295E+00 1.896135569397E+00
H -1.438150059709E+01 -2.946576424844E+00 7.636784354334E-01
H 1.581617930491E+01 -3.002447511730E+00 -5.008256378175E-01
H 1.117038239691E+01 -2.539168147459E+00 -1.678732408432E+00
H 6.524585488914E+00 -1.636843542874E+00 -2.566371094823E+00
H 1.878788580914E+00 -4.514938194695E-01 -3.010260904170E+00
H -2.767008327086E+00 8.119232870142E-01 -2.933649255824E+00
H -7.412805235086E+00 1.934951481082E+00 -2.349782999779E+00

H -1.205860214309E+01 2.723408985588E+00 -1.359617915964E+00
H -1.670439905109E+01 3.040964335092E+00 -1.343625427383E-01
H 1.349328085091E+01 2.832709324765E+00 1.114125334773E+00
H 8.847483942914E+00 2.134653137830E+00 2.169970820390E+00
H 4.201687034914E+00 1.067496030649E+00 2.850608637597E+00
H -1.210251593866E+00 1.398368022855E+00 2.884372181646E+00
H -5.856048501866E+00 1.042928968479E-01 3.203772620094E+00
H -1.050184540987E+01 -1.207815418495E+00 2.969211667167E+00
H -1.514764231787E+01 -2.311081475322E+00 2.221247042546E+00
H 1.505003758413E+01 -3.014740549550E+00 1.089208624873E+00
H 1.040424067613E+01 -3.197123594702E+00 -2.311638591908E-01
H 5.758443768134E+00 -2.826694925374E+00 -1.511566011942E+00
H 1.112646860134E+00 -1.967505023732E+00 -2.530604669083E+00
H -3.533150047866E+00 -7.681156292648E-01 -3.112078789118E+00
H -8.178946955866E+00 5.640879356140E-01 -3.155446214166E+00
H -1.282474386387E+01 1.798755571847E+00 -2.653208322455E+00
H 1.737293603813E+01 2.722402028526E+00 -1.692206608152E+00
H 1.272713913013E+01 3.175320442228E+00 -4.386069980841E-01
H 8.081342222134E+00 3.079197104587E+00 8.908317465717E-01
H 3.435545314134E+00 2.450652613936E+00 2.066237589293E+00
H 7.776124843228E-01 3.202467780373E+00 1.207704039269E-01
H -3.868184423677E+00 2.876478145330E+00 1.412890248472E+00
H -8.513981331677E+00 2.053119306977E+00 2.460708533352E+00
H -1.315977823968E+01 8.747574884432E-01 3.083047957980E+00
H 1.703790166232E+01 -4.548578467643E-01 3.172300382062E+00
H 1.239210475432E+01 -1.705824128013E+00 2.713033250641E+00
H 7.746307846323E+00 -2.661837920602E+00 1.784658023051E+00
H 3.100510938323E+00 -3.157595754680E+00 5.476992101660E-01
H -1.545285969677E+00 -3.107376596918E+00 -7.839617718475E-01
H -6.191082877677E+00 -2.519863795918E+00 -1.980068641439E+00
H -1.083687978568E+01 -1.496643652360E+00 -2.833803654568E+00
H -1.548267669368E+01 -2.146402247288E-01 -3.197548271523E+00
H 1.471500320832E+01 1.104476447704E+00 -3.008407743518E+00
H 1.006920630032E+01 2.232619108475E+00 -2.299086186132E+00
H 5.423409392323E+00 2.974721642683E+00 -1.192231740622E+00
H 5.468972397730E-01 1.275038387213E+00 2.999756209757E+00
H -4.098899668227E+00 -5.530524384396E-02 3.259018492866E+00
H -8.744696576227E+00 -1.376086095808E+00 2.954766871306E+00
H -1.339049348423E+01 -2.458929160457E+00 2.139609214482E+00
H 1.680718641777E+01 -3.116601034593E+00 9.544936867349E-01
H 1.216138950977E+01 -3.235384276416E+00 -3.956624707517E-01
H 7.515592601773E+00 -2.794740184304E+00 -1.677404992565E+00
H 2.869795693773E+00 -1.870860124908E+00 -2.669108952417E+00
H -1.776001214227E+00 -6.234913536842E-01 -3.199299726303E+00
H -6.421798122227E+00 7.316847368322E-01 -3.176302512786E+00

H -1.106759503023E+01 1.960345889203E+00 -2.604093739005E+00
H -1.571339193823E+01 2.850045428148E+00 -1.581613500302E+00
H 1.448428796377E+01 3.246946220715E+00 -2.856579188887E-01
H 9.838491055773E+00 3.082420514141E+00 1.059690511821E+00
H 5.192694147773E+00 2.384916297761E+00 2.221808826051E+00

PbE0/POB-TZVP optimized geometry, *all*-[148.9]-$(SnMe_2)_\infty$

Energy (a.u): -5.8218990557274E+02
Unit cell length (Å): 16.19042081

Sn	-2.197255041333E-01	6.938961844395E-01	4.521092792198E-01
Sn	-4.845560021276E+00	7.916392653675E-02	8.243954074785E-01
Sn	6.719026271581E+00	-5.951803826980E-01	5.758949793042E-01
Sn	2.093191754438E+00	-8.213417242939E-01	-1.062661144028E-01
Sn	-2.532642762705E+00	-4.290159951786E-01	-7.084066565309E-01
Sn	-7.158477279848E+00	2.863675286376E-01	-7.771025374288E-01
Sn	4.406109013010E+00	7.861104625567E-01	-2.606243576400E-01
C	1.581860551980E-02	2.712297396510E+00	-2.865355252548E-01
C	-4.610015911623E+00	1.915112260822E+00	1.941907516541E+00
C	6.954570381234E+00	-3.241914684361E-01	2.708054590687E+00
C	2.328735864091E+00	-2.319372409661E+00	1.434981323799E+00
C	-2.297098653052E+00	-2.568018619836E+00	-9.186621481939E-01
C	-6.922933170194E+00	-8.828944312413E-01	-2.580534285304E+00
C	4.641653122663E+00	1.467067271842E+00	-2.299211472274E+00
C	-4.547616365529E-01	8.338437949444E-01	2.596921056430E+00
C	-5.080596153696E+00	-1.510461536910E+00	2.271079125264E+00
C	6.483990139161E+00	-2.717358523671E+00	2.350682912033E-01
C	1.858155622019E+00	-1.878029118095E+00	-1.977953760653E+00
C	-2.767678895124E+00	3.754945182185E-01	-2.701536287834E+00
C	-7.393513412267E+00	2.346263123622E+00	-1.390806888979E+00
C	4.171072880590E+00	2.550247741892E+00	9.672284645682E-01
H	-8.796828498983E-01	3.298752383676E+00	-8.707426288718E-02
H	-5.505517367041E+00	2.124815870117E+00	2.524778551510E+00
H	6.059068925816E+00	-6.491503319848E-01	3.235421620523E+00
H	1.433234408673E+00	-2.934293093849E+00	1.509726218709E+00
H	-3.192600108470E+00	-3.009853307373E+00	-1.352823818595E+00
H	-7.818434625613E+00	-8.189325906276E-01	-3.196669927921E+00
H	3.746151667245E+00	1.988661070041E+00	-2.633358381339E+00
H	1.931604618343E-01	2.715870388211E+00	-1.360347998110E+00
H	-4.432674055309E+00	2.756880382254E+00	1.275189868006E+00
H	7.131912237549E+00	7.219032183491E-01	2.950483754380E+00
H	2.506077720406E+00	-1.856681793115E+00	2.404003194806E+00
H	-2.119756796737E+00	-3.037147544957E+00	4.725919681485E-02
H	-6.745591313880E+00	-1.930579248927E+00	-2.345071940290E+00
H	4.818994978977E+00	6.297545981849E-01	-2.971516075607E+00
H	-6.341257310410E-01	-1.466601326552E-01	3.033929821403E+00
H	-5.259960248184E+00	-2.463462947021E+00	1.776960794267E+00
H	6.304626044673E+00	-2.925227916794E+00	-8.180959543464E-01
H	1.678791527530E+00	-1.184236601446E+00	-2.797109763221E+00
H	-2.947042989612E+00	1.448509028815E+00	-2.669842869749E+00

H -7.572877506755E+00 2.990497816179E+00 -5.321298404867E-01
H 3.991708786102E+00 2.280580752922E+00 2.006287812133E+00
H -1.295493250522E+00 1.479334871532E+00 2.846297924495E+00
H -5.921327767665E+00 -1.302975119919E+00 2.931228304651E+00
H 5.643258525192E+00 -3.104118270223E+00 8.088839852439E-01
H 1.017424008049E+00 -2.567797050575E+00 -1.922566473278E+00
H -3.608410509094E+00 -9.787227833032E-02 -3.206285164213E+00
H 7.956175783763E+00 2.445752315728E+00 -2.075605730197E+00
H 3.330341266621E+00 3.147675531788E+00 6.180471532978E-01
H 8.579273940733E-01 3.200328290740E+00 2.016641488151E-01
H -3.767907123070E+00 1.837704671448E+00 2.627852952120E+00
H 7.796679169788E+00 -9.087480477885E-01 3.075214884048E+00
H 3.170844652645E+00 -2.970894951958E+00 1.206877285336E+00
H -1.454989864498E+00 -2.795897362090E+00 -1.570263525044E+00
H -6.080824381641E+00 -5.155320326561E-01 -3.164963873527E+00
H 5.483761911216E+00 2.153039432305E+00 -2.376381871747E+00
H 4.416511719002E-01 1.251335718723E+00 3.052752001947E+00
H -4.184183345243E+00 -1.606542563964E+00 2.881693400852E+00
H 7.380402947614E+00 -3.254661528490E+00 5.406608930829E-01
H 2.754568430472E+00 -2.451953979067E+00 -2.207500294650E+00
H -1.871266086671E+00 1.971249273397E-01 -3.293368735712E+00
H -6.497100603814E+00 2.697764742844E+00 -1.899263346303E+00
H 5.067485689043E+00 3.166932682615E+00 9.250260807834E-01

PbE0/POB-TZVP optimized geometry, *all*-[129.9]-$(SnMe_2)_\infty$

Energy (a.u): -1.0812104370381E+03
Unit cell length (Å): 29.77063381

Sn	-2.231565027616E-01	7.418776053666E-01	4.805773243175E-01
Sn	-1.167340027584E+01	4.335645773999E-01	7.702978016434E-01
Sn	6.646989761085E+00	2.592712977045E-02	8.835523357077E-01
Sn	-4.803254011992E+00	-3.876499108336E-01	7.943956776213E-01
Sn	1.351713602493E+01	-7.124210285536E-01	5.232525432975E-01
Sn	2.066892251854E+00	-8.739850742360E-01	1.322385571811E-01
Sn	-9.383351521223E+00	-8.353296720729E-01	-2.890696887382E-01
Sn	8.937038515700E+00	-6.053103088518E-01	-6.441555526350E-01
Sn	-2.513205257377E+00	-2.366216486527E-01	-8.516731423390E-01
Sn	-1.396344903045E+01	1.862741796527E-01	-8.640826789071E-01
Sn	4.356941006469E+00	5.664968382469E-01	-6.785412870628E-01
Sn	-7.093302766608E+00	8.169418982257E-01	-3.375542636614E-01
Sn	1.122708727032E+01	8.802354145382E-01	8.076237357503E-02
C	1.239538783618E-01	2.748550587609E+00	-2.482031290708E-01
C	-1.132628989472E+01	2.549066425064E+00	1.057542191375E+00
C	6.994100142208E+00	1.765621864117E+00	2.121017340541E+00
C	-4.456143630869E+00	5.776946121517E-01	2.698592978020E+00
C	1.386424640605E+01	-7.425755134832E-01	2.657953485805E+00
C	2.414002632977E+00	-1.892730537984E+00	2.008408881804E+00
C	-9.036241140100E+00	-2.609283806109E+00	8.987620069324E-01
C	9.284148896823E+00	-2.728081599532E+00	-4.167804124708E-01
C	-2.166094876254E+00	-2.221908775450E+00	-1.636843462125E+00
C	-1.361633864933E+01	-1.206723427816E+00	-2.481925400709E+00
C	4.704051387593E+00	8.490771453672E-02	-2.758428140434E+00
C	-6.746192385484E+00	1.357087522738E+00	-2.403008235848E+00
C	1.157419765144E+01	2.318374934158E+00	-1.497088103818E+00
C	-5.700250428079E-01	8.977976021780E-01	2.609833857233E+00
C	-1.202026881588E+01	-4.178899719750E-01	2.728120464378E+00
C	6.300121221038E+00	-1.637843989669E+00	2.221427550550E+00
C	-5.150122552039E+00	-2.482587687489E+00	1.205832355995E+00
C	1.317026748488E+01	-2.758600464531E+00	-8.600449946344E-02
C	1.720023711807E+00	-2.402651119888E+00	-1.358138760561E+00
C	-9.730220061269E+00	-1.496283358763E+00	-2.319139798961E+00
C	8.590169975654E+00	-2.471351123156E-01	-2.748853858083E+00
C	-2.860073797423E+00	1.058628810063E+00	-2.548838625598E+00
C	-1.431031757050E+01	2.121873629916E+00	-1.764915180824E+00
C	4.010072466423E+00	2.699022772504E+00	-5.766709376572E-01
C	-7.440171306654E+00	2.657858324663E+00	7.436816676890E-01
C	1.088021873027E+01	2.007810565306E+00	1.893665765303E+00
H	-7.380252324312E-01	3.381710177161E+00	-4.260485055254E-02

H -1.218826900551E+01 3.014155114673E+00 1.533834358819E+00
H 6.132121031415E+00 1.956093439921E+00 2.758890601293E+00
H -5.318122741662E+00 4.499143315638E-01 3.351918255247E+00
H 1.300226729526E+01 -1.159334728099E+00 3.177061831918E+00
H 1.552023522184E+00 -2.502994173052E+00 2.274378830642E+00
H -9.898220250893E+00 -3.273247817309E+00 8.506630485019E-01
H 8.422169786030E+00 -3.293639833533E+00 -7.679293864486E-01
H -3.028073987047E+00 -2.559498656557E+00 -2.210598453516E+00
H -1.447831776012E+01 -1.239007182667E+00 -3.146846055482E+00
H 3.842072276800E+00 3.653259051175E-01 -3.362189149744E+00
H -7.608171496277E+00 1.885967230694E+00 -2.807295228571E+00
H 1.071221854065E+01 2.974556192087E+00 -1.609283802107E+00
H 2.923831293652E-01 2.744535177123E+00 -1.323760795815E+00
H -1.115786064371E+01 3.045347526259E+00 1.033171201204E-01
H 7.162529393211E+00 2.648507457545E+00 1.506726328943E+00
H -4.287714379866E+00 1.644926248283E+00 2.564962693825E+00
H 1.403267565706E+01 2.645122590492E-01 3.035597016703E+00
H 2.582431883981E+00 -1.176498301014E+00 2.810812645964E+00
H -8.867811889096E+00 -2.347987278657E+00 1.942104972000E+00
H 9.452578147827E+00 -2.981580667074E+00 6.284844538522E-01
H -1.997665625250E+00 -2.932129856606E+00 -8.291142786141E-01
H -1.344790939833E+01 -2.210963431985E+00 -2.096772921760E+00
H 4.872480638596E+00 -9.832919300943E-01 -2.884086157384E+00
H -6.577763134481E+00 4.696399030288E-01 -3.010690011357E+00
H 1.174262690244E+01 1.814982894142E+00 -2.447581066476E+00
H -7.434332770437E-01 -8.473327585717E-02 3.045454420465E+00
H -1.219367705012E+01 -1.490320828274E+00 2.657238450719E+00
H 6.126712986802E+00 -2.554493839247E+00 1.660281175108E+00
H -5.323530786274E+00 -3.033463096636E+00 2.829734908369E-01
H 1.299685925065E+01 -2.817502515779E+00 -1.159160009985E+00
H 1.546615477572E+00 -1.956086063143E+00 -2.335743921911E+00
H -9.903628295505E+00 -6.465538668338E-01 -2.977237050094E+00
H 8.416761741418E+00 8.110960285483E-01 -2.936681049695E+00
H -3.033482031659E+00 2.082933598557E+00 -2.223366811655E+00
H -1.448372580474E+01 2.877596183207E+00 -1.000706031540E+00
H 3.836664232187E+00 3.013036161078E+00 4.512044405866E-01
H -7.613579540890E+00 2.458225865468E+00 1.799749412977E+00
H 1.070681049603E+01 1.340265648912E+00 2.735993484187E+00
H -1.438247184857E+00 1.521926889678E+00 2.813320760957E+00
H -1.288849095793E+01 4.018398706051E-02 3.198346511675E+00
H 5.431899078989E+00 -1.450764582723E+00 2.850669620821E+00
H -6.018344694088E+00 -2.609360470213E+00 1.849938674131E+00
H 1.230204534283E+01 -3.170183320180E+00 4.254090713750E-01
H 8.518015697580E-01 -3.004755376344E+00 -1.096576622898E+00
H -1.059844220332E+01 -2.150974187016E+00 -2.367349828046E+00

H 7.721947833604E+00 -8.044307334911E-01 -3.095791717246E+00
H -3.728295939473E+00 7.263981066352E-01 -3.115025032361E+00
H 1.459209409745E+01 2.090817894578E+00 -2.420643652682E+00
H 3.141850324373E+00 2.976256499959E+00 -1.171721984093E+00
H -8.308393448704E+00 3.179870608980E+00 3.456270702718E-01
H 1.001199658822E+01 2.655014683078E+00 1.783797128095E+00
H 9.951877393591E-01 3.187760736808E+00 2.342593620883E-01
H -1.045505603372E+01 2.713756198917E+00 1.688852645053E+00
H 7.865334003205E+00 1.618062820161E+00 2.756550139916E+00
H -3.584909769872E+00 1.516907490775E-01 3.192755217756E+00
H 1.473548026705E+01 -1.349431844548E+00 2.897538552078E+00
H 3.285236493974E+00 -2.541415865004E+00 1.938530723245E+00
H -8.165007279102E+00 -3.151192138170E+00 5.354288675439E-01
H 1.015538275782E+01 -3.039068268462E+00 -9.903332890941E-01
H -1.294861015256E+00 -2.230730483193E+00 -2.289222024011E+00
H -1.274510478833E+01 -9.113592274407E-01 -3.063677581342E+00
H 5.575285248590E+00 6.167934442487E-01 -3.136281526106E+00
H -5.874958524487E+00 2.003646171028E+00 -2.490401169528E+00
H 1.244543151244E+01 2.931487706578E+00 -1.273999917599E+00
H 2.939556867427E-01 1.339897304315E+00 3.104054773053E+00
H -1.115628808633E+01 -2.561060384686E-01 3.371185328232E+00
H 7.164101950589E+00 -1.793438574251E+00 2.866017951900E+00
H -4.286141822488E+00 -2.919915945951E+00 1.704280402048E+00
H 1.403424821443E+01 -3.377475763235E+00 1.521127508926E-01
H 2.584004441358E+00 -3.061296586157E+00 -1.434902098335E+00
H -8.866239331719E+00 -2.043811253814E+00 -2.693198169279E+00
H 9.454150705204E+00 -5.581133938177E-01 -3.334514996197E+00
H -1.996093067873E+00 1.055441518707E+00 -3.211934622749E+00
H -1.344633684095E+01 2.427207498745E+00 -2.353538735237E+00
H 4.874053195973E+00 3.242929491841E+00 -9.559754866991E-01
H -6.576190577103E+00 3.315735419894E+00 6.605902250883E-01
H 1.174419945982E+01 2.628946322193E+00 2.125822677283E+00

PbE0/POB-TZVP optimized geometry, *all*-[−118.8]-$(SnMe_2)_\infty$

Energy (a.u): -9.1486776955242E+02
Unit cell length (Å): 24.922134870

Sn	-2.247183143958E-01	7.776499966028E-01	5.036037924722E-01
Sn	-7.021664188032E+00	3.819320409124E-01	8.440877994221E-01
Sn	1.110352480833E+01	-1.350466391649E-01	9.165798940949E-01
Sn	4.306578934695E+00	-6.091489655013E-01	6.980643486366E-01
Sn	-2.490366938941E+00	-8.898507993319E-01	2.579183047732E-01
Sn	-9.287312812578E+00	-8.880312917600E-01	-2.641149784921E-01
Sn	8.837876183786E+00	-6.042681235835E-01	-7.022936222333E-01
Sn	2.040930310150E+00	-1.286540957238E-01	-9.174990030851E-01
Sn	-4.756015563487E+00	3.878066985018E-01	-8.414049331956E-01
Sn	-1.155296143712E+01	7.811416060643E-01	-4.981707420996E-01
Sn	6.572227559241E+00	9.264695729842E-01	3.229139706739E-03
C	-6.399177402505E-01	2.777015944905E+00	-2.099979305402E-01
C	-7.436863613887E+00	2.449707927211E+00	1.324706669586E+00
C	1.068832538248E+01	1.344634951437E+00	2.438826262050E+00
C	3.891379508840E+00	-1.873501206822E-01	2.778635748235E+00
C	-2.905566364796E+00	-1.659852853237E+00	2.236248017257E+00
C	-9.702512238432E+00	-2.605364032849E+00	9.838673413744E-01
C	8.422676757931E+00	-2.723690540654E+00	-5.808842637206E-01
C	1.625730884295E+00	-1.977264546479E+00	-1.961209219416E+00
C	-5.171214989341E+00	-6.030710294808E-01	-2.718864105190E+00
C	-1.196816086298E+01	9.625932782816E-01	-2.613298848141E+00
C	6.157028133386E+00	2.222641021549E+00	-1.678029671495E+00
C	1.910989437767E-01	9.443416003384E-01	2.619825716218E+00
C	-6.605846929860E+00	-6.219540093232E-01	2.714487253935E+00
C	1.151934206650E+01	-1.990783615542E+00	1.947318268177E+00
C	4.722396192868E+00	-2.727553490031E+00	5.618894913673E-01
C	-2.074549680769E+00	-2.598344403407E+00	-1.001935228830E+00
C	-8.871495554405E+00	-1.644179327726E+00	-2.247652593211E+00
C	9.253693441958E+00	-1.679989327075E-01	-2.779756140401E+00
C	2.456747568322E+00	1.361519936421E+00	-2.429306753832E+00
C	-4.340198305314E+00	2.458765845777E+00	-1.307569637583E+00
C	-1.113714417895E+01	2.775370971907E+00	2.293115997533E-01
C	6.988044817413E+00	2.210815424291E+00	1.693388024406E+00
H	-1.536651345282E+00	3.178294352946E+00	2.586724854759E-01
H	-8.333597218918E+00	2.533902448792E+00	1.935924799344E+00
H	9.791591777446E+00	1.085014420846E+00	2.998534668011E+00
H	2.994645903809E+00	-7.083580193731E-01	3.109130966219E+00
H	-3.802299969827E+00	-2.276831793460E+00	2.232600150721E+00
H	-1.059924584346E+01	-3.122427560448E+00	6.472345621686E-01
H	7.525943152900E+00	-2.976674639013E+00	-1.143623426732E+00

H 7.289972792638E-01 -1.885848551869E+00 -2.571389058102E+00
H -6.067948594373E+00 -1.962788742757E-01 -3.182756832091E+00
H 1.205724040199E+01 1.555607959060E+00 -2.783621800177E+00
H 5.260294528355E+00 2.813600256794E+00 -1.500706514838E+00
H -7.876505346277E-01 2.779956649391E+00 -1.288284679459E+00
H -7.584596408264E+00 3.035147634636E+00 4.191839975307E-01
H 1.054059258810E+01 2.326700691212E+00 1.993564717117E+00
H 3.743646714463E+00 8.795427180104E-01 2.935002724874E+00
H -3.053299159173E+00 -8.468638536080E-01 2.944598105222E+00
H -9.850245032809E+00 -2.304397135360E+00 2.019304392697E+00
H 8.274943963554E+00 -3.030300608727E+00 4.528958032149E-01
H 1.477998089918E+00 -2.794105049905E+00 -1.257304003780E+00
H -5.318947783719E+00 -1.670800879940E+00 -2.568318673260E+00
H -1.211589365735E+01 -1.702923590950E-02 -3.063910310852E+00
H 6.009295339009E+00 1.642149070199E+00 -2.586732073305E+00
H 3.401600129904E-01 -3.830953629045E-02 3.063350596106E+00
H -6.456785860646E+00 -1.688400403177E+00 2.556342812258E+00
H 1.166840313572E+01 -2.802436071723E+00 1.237714247774E+00
H 4.871457262081E+00 -3.026718088563E+00 -4.738798451080E-01
H -1.925488611555E+00 -2.290038498053E+00 -2.035020435443E+00
H -8.722434485191E+00 -8.262878650495E-01 -2.950056416292E+00
H 9.402754511172E+00 8.998033268358E-01 -2.928470329071E+00
H 2.605808637536E+00 2.340213320157E+00 -1.977115603952E+00
H -4.191137236100E+00 3.037622119486E+00 -3.980406442104E-01
H -1.098808310974E+01 2.770607358690E+00 1.307409407648E+00
H 7.137105886627E+00 1.623944337686E+00 2.597766210291E+00
H -6.421332472529E-01 1.424664272970E+00 3.130965823046E+00
H -7.439079120889E+00 -4.942240692627E-01 3.404167716949E+00
H 1.068610987547E+01 -2.256199761525E+00 2.596570413421E+00
H 3.889164001838E+00 -3.301847971049E+00 9.645803501214E-01
H -2.907781871798E+00 -3.299182779508E+00 -9.736571589427E-01
H -9.704727745435E+00 -2.249050366384E+00 -2.602765399575E+00
H 8.420461250929E+00 -4.848603529644E-01 -3.405514016104E+00
H 1.623515377293E+00 1.433269396662E+00 -3.127035994732E+00
H -5.173430496344E+00 2.896346239846E+00 -1.855746139613E+00
H -1.197037636998E+01 3.439853616483E+00 4.730002757119E-03
H 6.154812626384E+00 2.891231774732E+00 1.863704402673E+00
H 1.931018155489E-01 3.439833409499E+00 2.028342480654E-02
H -6.603844058087E+00 2.882805960724E+00 1.876777849199E+00
H 1.152134493828E+01 1.410507988352E+00 3.137408567149E+00
H 4.724399064640E+00 -5.096163041482E-01 3.401934232900E+00
H -2.072546808997E+00 -2.267941020858E+00 2.586369816623E+00
H -8.869492682633E+00 -3.306210487951E+00 9.496512579840E-01
H 9.255696313731E+00 -3.294781485686E+00 -9.885748651494E-01
H 2.458750440094E+00 -2.237282641530E+00 -2.612935453534E+00

H -4.338195433542E+00 -4.694623665716E-01 -3.407707497541E+00
H -1.113514130718E+01 1.447408892711E+00 -3.120556488790E+00
H 6.990047689185E+00 2.904738055460E+00 -1.842650843646E+00
H 1.087306257137E+00 1.537078199429E+00 2.793865495849E+00
H -5.709639616499E+00 -2.174052600294E-01 3.181356432871E+00
H 1.241554937986E+01 -1.902864085541E+00 2.558789180846E+00
H 5.618603506228E+00 -2.984177008888E+00 1.123824443443E+00
H -1.178342367408E+00 -3.118034817100E+00 -6.679466141884E-01
H -7.975288241044E+00 -2.261938601865E+00 -2.247649341301E+00
H 1.014990075532E+01 -6.876928626316E-01 -3.113739283681E+00
H 3.352954881683E+00 1.104890501482E+00 -2.991239004124E+00
H -3.443990991954E+00 2.546678938158E+00 -1.919041475842E+00
H -1.024093686559E+01 3.179914805942E+00 -2.375618382789E-01
H 7.884252130774E+00 2.803550191044E+00 1.519342004406E+00

PbE0/POB-TZVP optimized geometry, *all*-[−99.7]-$(SnMe_2)_\infty$

Energy (a.u): -2.0792489416389E+03
Unit cell length (Å): 52.9836717000

Sn	-2.189051063952E-01	9.232685492259E-01	5.978788650500E-01
Sn	6.139135497605E+00	7.455759424923E-01	8.087029524120E-01
Sn	1.249717610160E+01	5.210360572555E-01	9.687132590725E-01
Sn	1.885521670560E+01	2.637575603047E-01	1.067855748987E+00
Sn	2.521325730960E+01	-1.009379419254E-02	1.099900934895E+00
Sn	-2.141237378640E+01	-2.833109184782E-01	1.062835299910E+00
Sn	-1.505433318240E+01	-5.387265758113E-01	9.589878141967E-01
Sn	-8.696292578395E+00	-7.602920610884E-01	7.948835972073E-01
Sn	-2.338251974395E+00	-9.340856000086E-01	5.808339204279E-01
Sn	4.019788629605E+00	-1.049187105354E+00	3.302883122704E-01
Sn	1.037782923360E+01	-1.098364326229E+00	5.898947473740E-02
Sn	1.673586983760E+01	-1.078527276987E+00	-2.160158884414E-01
Sn	2.309391044160E+01	-9.909223923848E-01	-4.774481788986E-01
Sn	-2.353172065440E+01	-8.410542095118E-01	-7.088806443440E-01
Sn	-1.717368005040E+01	-6.383394974742E-01	-8.957715318247E-01
Sn	-1.081563944640E+01	-3.955155671619E-01	-1.026377799544E+00
Sn	-4.457598842395E+00	-1.278399391603E-01	-1.092492975364E+00
Sn	1.900441761605E+00	1.478683423812E-01	-1.089962799633E+00
Sn	8.258482365605E+00	4.142855121491E-01	-1.018946252599E+00
Sn	1.461652296960E+01	6.546715995532E-01	-8.839055650926E-01
Sn	2.097456357360E+01	8.539222626437E-01	-6.933258401536E-01
Sn	-2.565106752240E+01	9.995178494658E-01	-4.591819028037E-01
Sn	-1.929302691840E+01	1.082310053836E+00	-1.961858777478E-01
Sn	-1.293498631440E+01	1.097096737067E+00	7.913722752822E-02
Sn	-6.576945710395E+00	1.042948797467E+00	3.494878497523E-01
C	-9.297522020023E-01	2.865709914218E+00	-3.607006284726E-02
C	5.428288401998E+00	2.784648627450E+00	6.777362197194E-01
C	1.178632900600E+01	2.528617626199E+00	1.348957843062E+00
C	1.814436961000E+01	2.113704279888E+00	1.935419484004E+00
C	2.450241021400E+01	1.565979120012E+00	2.400271600792E+00
C	-2.212322088200E+01	9.198577327562E-01	2.714305825321E+00
C	-1.576518027800E+01	2.159383011517E-01	2.857790232326E+00
C	-9.407139674002E+00	-5.015493280797E-01	2.821709168817E+00
C	-3.049099070002E+00	-1.187522768458E+00	2.608329740710E+00
C	3.308941533998E+00	-1.798879785892E+00	2.231059362229E+00
C	9.666982137998E+00	-2.297206570560E+00	1.713603318757E+00
C	1.602502274200E+01	-2.651191417866E+00	1.088475276575E+00
C	2.238306334600E+01	-2.838592157987E+00	3.949543296343E-01
C	-2.424256775000E+01	-2.847633713210E+00	-3.233830503781E-01
C	-1.788452714600E+01	-2.677747969368E+00	-1.021401084016E+00

C -1.152648654200E+01 -2.339609472542E+00 -1.655240731094E+00
C -5.168445938002E+00 -1.854464708075E+00 -2.185075515488E+00
C 1.189594665998E+00 -1.252797105755E+00 -2.577613969099E+00
C 7.547635269998E+00 -5.724116538154E-01 -2.808191457230E+00
C 1.390567587400E+01 1.439405275164E-01 -2.862319948297E+00
C 2.026371647800E+01 8.512483961281E-01 -2.736598350137E+00
C -2.636191461800E+01 1.505069197338E+00 -2.438926213132E+00
C -2.000387401400E+01 2.064320965623E+00 -1.988007372414E+00
C -1.364583341000E+01 2.493863855595E+00 -1.412174717107E+00
C -7.287792806002E+00 2.766708107731E+00 -7.476099307088E-01
C 4.920664817549E-01 1.139314324383E+00 2.629653675570E+00
C 6.850107085755E+00 4.495523939699E-01 2.830374220533E+00
C 1.320814768975E+01 -2.684565666944E-01 2.853251943832E+00
C 1.956618829375E+01 -9.695974139592E-01 2.696849353973E+00
C 2.592422889775E+01 -1.609814889775E+00 2.370993800886E+00
C -2.070140219825E+01 -2.148881775581E+00 1.896159987385E+00
C -1.434336159425E+01 -2.552926516393E+00 1.302183468287E+00
C -7.985320990245E+00 -2.796561495173E+00 6.263859727805E-01
C -1.627280386245E+00 -2.864478230178E+00 -8.876965708190E-02
C 4.730760217755E+00 -2.752409263167E+00 -7.983475629179E-01
C 1.108880082175E+01 -2.467396299497E+00 -1.457762355259E+00
C 1.744684142575E+01 -2.027347751882E+00 -2.025580577544E+00
C 2.380488202975E+01 -1.459913488952E+00 -2.466124122578E+00
C -2.282074906625E+01 -8.007474923251E-01 -2.751712019220E+00
C -1.646270846225E+01 -9.126758581215E-02 -2.864399729605E+00
C -1.010466785825E+01 6.239469987761E-01 -2.797106670455E+00
C -3.746627254245E+00 1.299956698715E+00 -2.554061112160E+00
C 2.611413349755E+00 1.894285338367E+00 -2.150534501009E+00
C 8.969453953755E+00 2.369589063515E+00 -1.611881898047E+00
C 1.532749455775E+01 2.696002793064E+00 -9.719488273442E-01
C 2.168553516175E+01 2.853016751920E+00 -2.709446372412E-01
C -2.494009593425E+01 2.830765175591E+00 4.470840008844E-01
C -1.858205533025E+01 2.630646212453E+00 1.137020706974E+00
C -1.222401472625E+01 2.265234072947E+00 1.755514220376E+00
C -5.865974122245E+00 1.757488945690E+00 2.263702318981E+00
H -1.785465912587E+00 3.176503541006E+00 5.618292961601E-01
H 4.572574691413E+00 2.936986576816E+00 1.334142702881E+00
H 1.093061529541E+01 2.512927944523E+00 2.022627016946E+00
H 1.728865589941E+01 1.930972807574E+00 2.584022236835E+00
H 2.364669650341E+01 1.227687547504E+00 2.983053836214E+00
H -2.297893459259E+01 4.472621637045E-01 3.194649192160E+00
H -1.662089398859E+01 -3.612663467554E-01 3.205512990264E+00
H -1.026285338459E+01 -1.147095164004E+00 3.014962618137E+00
H -3.904812780587E+00 -1.860847773377E+00 2.634971056457E+00
H 2.453227823413E+00 -2.457676473430E+00 2.089414572553E+00

H 8.811268427413E+00 -2.900080321955E+00 1.412572486727E+00
H 1.516930903141E+01 -3.160261458102E+00 6.469732764813E-01
H 2.152734963541E+01 -3.221871744208E+00 -1.592776441269E-01
H -2.509828146059E+01 -3.081039979411E+00 -9.555205645723E-01
H -1.874024085659E+01 -2.746615141434E+00 -1.691724613787E+00
H -1.238220025259E+01 -2.239610372777E+00 -2.321631383789E+00
H -6.024159648587E+00 -1.591882647688E+00 -2.805661515585E+00
H 3.338809554132E-01 -8.441310813099E-01 -3.113401615856E+00
H 6.691921559413E+00 -4.333965459597E-02 -3.225515242312E+00
H 1.304996216341E+01 7.601749620083E-01 -3.134957883478E+00
H 1.940800276741E+01 1.515924990022E+00 -2.847419591257E+00
H 2.576604337141E+01 2.176423875730E+00 -2.380967454041E+00
H -2.085958772459E+01 2.700170044999E+00 -1.764910375101E+00
H -1.450154712059E+01 3.054254599810E+00 -1.037957486407E+00
H -8.143506516587E+00 3.216429105352E+00 -2.457859115021E-01
H -1.231695311107E+00 2.841626202684E+00 -1.081317869284E+00
H 5.126345292893E+00 3.021264109043E+00 -3.406625803058E-01
H 1.148438589689E+01 3.011064879999E+00 4.213977914624E-01
H 1.784242650089E+01 2.811669370623E+00 1.156980190200E+00
H 2.420046710489E+01 2.435606334093E+00 1.819865268512E+00
H -2.242516399111E+01 1.906505194059E+00 2.368401519008E+00
H -1.606712338711E+01 1.257611321047E+00 2.768122391692E+00
H -9.709082783107E+00 5.296971035626E-01 2.993911954065E+00
H -3.351042179107E+00 -2.314999310285E-01 3.031583017525E+00
H 3.006998424893E+00 -9.781509735558E-01 2.878768570612E+00
H 9.365039028893E+00 -1.663341193027E+00 2.545070507038E+00
H 1.572307963289E+01 -2.244017567999E+00 2.051456303391E+00
H 2.208112023689E+01 -2.683694066255E+00 1.428941555474E+00
H -2.454451085911E+01 -2.954744196391E+00 7.166411543473E-01
H -1.818647025511E+01 -3.040136881880E+00 -4.068844612906E-02
H -1.182842965111E+01 -2.934506586238E+00 -7.954614418935E-01
H -5.470389047107E+00 -2.644490449423E+00 -1.500252669761E+00
H 8.876515568927E-01 -2.188311251915E+00 -2.110777504844E+00
H 7.245692160893E+00 -1.594632410403E+00 -2.588674426402E+00
H 1.360373276489E+01 -9.007569498979E-01 -2.903915413269E+00
H 1.996177336889E+01 -1.502836174784E-01 -3.036692714868E+00
H 2.631981397289E+01 6.096325873317E-01 -2.978663445016E+00
H -2.030581712311E+01 1.331243334608E+00 -2.733473796157E+00
H -1.394777651911E+01 1.969207167200E+00 -2.316529935671E+00
H -7.589735915107E+00 2.483438471240E+00 -1.754029979726E+00
H 7.939310283057E-01 1.756491409048E-01 3.035258096373E+00
H 7.151971632306E+00 -5.847071933561E-01 2.983582046858E+00
H 1.351001223631E+01 -1.308324224256E+00 2.744436564493E+00
H 1.986805284031E+01 -1.949734432466E+00 2.332848039448E+00
H 2.622609344431E+01 -2.468635655662E+00 1.774678092470E+00

H -2.039953765169E+01 -2.832423421606E+00 1.104998594133E+00
H -1.404149704769E+01 -3.018239607046E+00 3.658879702253E-01
H -7.683456443694E+00 -3.014408697667E+00 -3.962127404931E-01
H -1.325415839694E+00 -2.821171403593E+00 -1.133417947558E+00
H 5.032624764306E+00 -2.450669534689E+00 -1.799406336558E+00
H 1.139066536831E+01 -1.926183085989E+00 -2.352331407678E+00
H 1.774870597231E+01 -1.280667469990E+00 -2.757450845185E+00
H 2.410674657631E+01 -5.546828068856E-01 -2.989309504893E+00
H -2.251888451969E+01 2.061546169558E-01 -3.033338854498E+00
H -1.616084391569E+01 9.540385880301E-01 -2.886772368035E+00
H -9.802803311694E+00 1.641976805910E+00 -2.558819356882E+00
H -3.444762707694E+00 2.226743582306E+00 -2.070086314856E+00
H 2.913277896306E+00 2.671595870036E+00 -1.451282136424E+00
H 9.271318500306E+00 2.948581963810E+00 -7.412885639176E-01
H 1.562935910431E+01 3.040297808671E+00 1.528289532836E-02
H 2.198739970831E+01 2.940980560780E+00 7.708940740543E-01
H -2.463823138769E+01 2.656870688086E+00 1.478067142957E+00
H -1.828019078369E+01 2.205819858772E+00 2.092367817318E+00
H -1.192215017969E+01 1.616169255294E+00 2.575197326525E+00
H -5.564109575694E+00 9.249687936503E-01 2.896217716794E+00
H -2.919465685335E-01 1.546758006792E+00 3.266110122552E+00
H 6.066094035466E+00 6.859152018742E-01 3.548162341276E+00
H 1.242413463947E+01 -2.180261777971E-01 3.607270470869E+00
H 1.878217524347E+01 -1.108268170873E+00 3.439720530165E+00
H 2.514021584747E+01 -1.928873598848E+00 3.056040298144E+00
H -2.148541524853E+01 -2.628280804706E+00 2.480337814860E+00
H -1.512737464453E+01 -3.162543461464E+00 1.748786584624E+00
H -8.769334040534E+00 -3.498091881517E+00 9.073526616888E-01
H -2.411293436534E+00 -3.613842323573E+00 8.906434010117E-03
H 3.946747167466E+00 -3.502521761655E+00 -8.900994176730E-01
H 1.030478777147E+01 -3.171124876079E+00 -1.733177049387E+00
H 1.666282837547E+01 -2.640474551958E+00 -2.467352792909E+00
H 2.302086897947E+01 -1.943913500751E+00 -3.046495686163E+00
H -2.360476211653E+01 -1.125209215078E+00 -3.434216051229E+00
H -1.724672151253E+01 -2.358038961912E-01 -3.606151991632E+00
H -1.088868090853E+01 6.684178487190E-01 -3.551500139902E+00
H -4.530640304534E+00 1.530640441925E+00 -3.273694472878E+00
H 1.827400299466E+00 2.296687266864E+00 -2.790190542318E+00
H 8.185440903467E+00 2.918424784200E+00 -2.131368678380E+00
H 1.454348150747E+01 3.356786939130E+00 -1.338625081754E+00
H 2.090152211147E+01 3.584229825275E+00 -4.617707481226E-01
H -2.572410898453E+01 3.586462369623E+00 4.440983398872E-01
H -1.936606838053E+01 3.363344293202E+00 1.322063095922E+00
H -1.300802777653E+01 2.928894925323E+00 2.116957765433E+00
H -6.649987172534E+00 2.310412317565E+00 2.778836192915E+00

H -1.456566701327E-01 3.613076470931E+00 7.527924360837E-02
H 6.212383933867E+00 3.480843843015E+00 9.714497876154E-01
H 1.257042453787E+01 3.129896994794E+00 1.806580568724E+00
H 1.892846514187E+01 2.582287207435E+00 2.528197248561E+00
H 2.528650574587E+01 1.872422817844E+00 3.090957997212E+00
H -2.133912535013E+01 1.044907216318E+00 3.459502487150E+00
H -1.498108474613E+01 1.517362514919E-01 3.610673712660E+00
H -8.623044142133E+00 -7.509688600628E-01 3.534973029675E+00
H -2.265003538133E+00 -1.606487836269E+00 3.237156990514E+00
H 4.093037065867E+00 -2.361065273474E+00 2.735938472208E+00
H 1.045107766987E+01 -2.967288296156E+00 2.062810877615E+00
H 1.680911827387E+01 -3.387065682268E+00 1.260069289094E+00
H 2.316715887787E+01 -3.594021274806E+00 3.781529129292E-01
H -2.345847221813E+01 -3.575151292762E+00 -5.275242015046E-01
H -1.710043161413E+01 -3.331641406508E+00 -1.400055030260E+00
H -1.074239101013E+01 -2.878792237763E+00 -2.184615252421E+00
H -4.384350406133E+00 -2.245057965262E+00 -2.831908063820E+00
H 1.973690197867E+00 -1.470258444057E+00 -3.301261676540E+00
H 8.331730801867E+00 -6.030771775808E-01 -3.563184876932E+00
H 1.468977140587E+01 3.019976459259E-01 -3.601220067028E+00
H 2.104781200987E+01 1.188096846669E+00 -3.412977355953E+00
H -2.557781908613E+01 1.999543553022E+00 -3.010284725550E+00
H -1.921977848213E+01 2.685351584132E+00 -2.418444834788E+00
H -1.286173787813E+01 3.202429099178E+00 -1.674645160639E+00
H -6.503697274133E+00 3.518286216213E+00 -8.256213721323E-01
H 1.347860696067E+00 1.811957928777E+00 2.668585116394E+00
H 7.705901300067E+00 1.091381807001E+00 3.035362220633E+00
H 1.406394190407E+01 3.022301524698E-01 3.211416353268E+00
H 2.042198250807E+01 -5.059117340660E-01 3.185685385664E+00
H -2.620364858793E+01 -1.282265325737E+00 2.959786089147E+00
H -1.984560798393E+01 -1.978049471150E+00 2.547912547318E+00
H -1.348756737993E+01 -2.549545493534E+00 1.975944289574E+00
H -7.129526775933E+00 -2.960844195986E+00 1.279820185101E+00
H -7.714861719327E-01 -3.186102168382E+00 5.032802715484E-01
H 5.586554432067E+00 -3.211165623874E+00 -3.048825924006E-01
H 1.194459503607E+01 -3.034459733377E+00 -1.093888561789E+00
H 1.830263564007E+01 -2.667087577869E+00 -1.814161489800E+00
H 2.466067624407E+01 -2.132132500982E+00 -2.420443979387E+00
H -2.196495485193E+01 -1.463207697624E+00 -2.874641071980E+00
H -1.560691424793E+01 -7.023441733221E-01 -3.148213893829E+00
H -9.248873643933E+00 1.026502184306E-01 -3.223972858408E+00
H -2.890833039933E+00 9.011947194381E-01 -3.097157751351E+00
H 3.467207564067E+00 1.643113841861E+00 -2.775736832227E+00
H 9.825248168067E+00 2.281790078650E+00 -2.279906159488E+00
H 1.618328877207E+01 2.777093052960E+00 -1.640820597840E+00

H 2.254132937607E+01 3.097901057319E+00 -8.986362435142E-01
H -2.408430171993E+01 3.224056544964E+00 -9.998726905516E-02
H -1.772626111593E+01 3.147632702638E+00 7.049442732461E-01
H -1.136822051193E+01 2.873431521422E+00 1.465581574256E+00
H -5.010179907933E+00 2.418682069973E+00 2.134130994923E+00

PbE0/POB-TZVP optimized geometry, *all*-[87.3]-$(SnMe_2)_\infty$

Energy (a.u): -8.3170323768959E+02
Unit cell length (Å): 19.5316795200

SN	-2.088170475629E-01	1.062673662617E+00	6.673099481459E-01
SN	-6.068320903563E+00	4.674861063036E-01	1.164488995451E+00
SN	7.603854760437E+00	-3.062652533494E-01	1.216872826020E+00
SN	1.744350904437E+00	-9.630336957961E-01	8.044525970346E-01
SN	-4.115152951563E+00	-1.251955998760E+00	8.475881832040E-02
SN	9.557022712437E+00	-1.062673662617E+00	-6.673099481459E-01
SN	3.697518856437E+00	-4.674861063036E-01	-1.164488995451E+00
SN	-2.161984999563E+00	3.062652533494E-01	-1.216872826020E+00
SN	-8.021488855563E+00	9.630336957961E-01	-8.044525970346E-01
SN	5.650686808437E+00	1.251955998760E+00	-8.475881832040E-02
C	7.354831561961E-01	2.930689737665E+00	1.206550026746E-01
C	-5.124020699804E+00	2.300058571824E+00	1.820228154464E+00
C	8.548154964196E+00	7.908832076615E-01	2.824536018528E+00
C	2.688651108196E+00	-1.020382660696E+00	2.749967125963E+00
C	-3.170852747804E+00	-2.441897034199E+00	1.625004259224E+00
C	-9.030356603804E+00	-2.930689737665E+00	-1.206550026746E-01
C	4.641819060196E+00	-2.300058571824E+00	-1.820228154464E+00
C	-1.217684795804E+00	-7.908832076615E-01	-2.824536018528E+00
C	-7.077188651804E+00	1.020382660696E+00	-2.749967125963E+00
C	6.594987012196E+00	2.441897034199E+00	-1.625004259224E+00
C	-1.152184191652E+00	1.382614730349E+00	2.587649268003E+00
C	-7.011688047652E+00	-4.024232643121E-01	2.906132781398E+00
C	6.660487616348E+00	-2.033749249870E+00	2.114572348119E+00
C	8.009837603484E-01	-2.888252146572E+00	5.153171495293E-01
C	-5.058520095652E+00	-2.639540891363E+00	-1.280771685195E+00
C	8.613655568348E+00	-1.382614730349E+00	-2.587649268003E+00
C	2.754151712348E+00	4.024232643121E-01	-2.906132781398E+00
C	-3.105352143652E+00	2.033749249870E+00	-2.114572348119E+00
C	-8.964855999652E+00	2.888252146572E+00	-5.153171495293E-01
C	4.707319664348E+00	2.639540891363E+00	1.280771685195E+00
H	-5.418827018680E-03	3.722510647206E+00	2.332488314283E-02
H	-5.864922683019E+00	2.997864353009E+00	2.206907086784E+00
H	7.807252980981E+00	1.128135769624E+00	3.547525793286E+00
H	1.947749124981E+00	-1.172502333833E+00	3.533110222720E+00
H	-3.911754731019E+00	-3.025284397654E+00	2.169166633075E+00
H	9.760420932981E+00	-3.722510647206E+00	-2.332488314283E-02
H	3.900917076981E+00	-2.997864353009E+00	-2.206907086784E+00
H	-1.958586779019E+00	-1.128135769624E+00	-3.547525793286E+00
H	-7.818090635019E+00	1.172502333833E+00	-3.533110222720E+00
H	5.854085028981E+00	3.025284397654E+00	-2.169166633075E+00

H 1.262631091788E+00 2.838606563564E+00 -8.273165238068E-01
H -4.596872764212E+00 2.782765401939E+00 9.991779476366E-01
H 9.075302899788E+00 1.664002439491E+00 2.444020403892E+00
H 3.215799043788E+00 -9.035289748043E-02 2.955330135059E+00
H -2.643704812212E+00 -1.810196498596E+00 2.337804202610E+00
H -8.503208668212E+00 -2.838606563564E+00 8.273165238068E-01
H 5.168966995788E+00 -2.782765401939E+00 -9.991779476366E-01
H -6.905368602116E-01 -1.664002439491E+00 -2.444020403892E+00
H -6.550040716212E+00 9.035289748043E-02 -2.955330135059E+00
H 7.122134947788E+00 1.810196498596E+00 -2.337804202610E+00
H -1.682814612171E+00 4.903171121627E-01 2.915126648585E+00
H -7.542318468171E+00 -1.316793576231E+00 2.646588166936E+00
H 6.129857195829E+00 -2.620933874671E+00 1.367142959741E+00
H 2.703533398291E-01 -2.923966515254E+00 -4.345043905947E-01
H -5.589150516171E+00 -2.110143328976E+00 -2.070185831985E+00
H 8.083025147829E+00 -4.903171121627E-01 -2.915126648585E+00
H 2.223521291829E+00 1.316793576231E+00 -2.646588166936E+00
H -3.635982564171E+00 2.620933874671E+00 -1.367142959741E+00
H -9.495486420171E+00 2.923966515254E+00 4.345043905947E-01
H 4.176689243829E+00 2.110143328976E+00 2.070185831985E+00
H -1.866282795430E+00 2.202211291825E+00 2.520756650658E+00
H -7.725786651430E+00 2.999627764159E-01 3.333762288833E+00
H 5.946389012570E+00 -1.716861324224E+00 2.873384043086E+00
H 8.688515656988E-02 -3.077902752981E+00 1.315470755612E+00
H -5.772618699430E+00 -3.263289944166E+00 -7.449076492993E-01
H 7.899556964570E+00 -2.202211291825E+00 -2.520756650658E+00
H 2.040053108570E+00 -2.999627764159E-01 -3.333762288833E+00
H -3.819450747430E+00 1.716861324224E+00 -2.873384043086E+00
H -9.678954603430E+00 3.077902752981E+00 -1.315470755612E+00
H 3.993221060570E+00 3.263289944166E+00 7.449076492993E-01
H 1.452790418216E+00 3.224261983808E+00 8.857890011812E-01
H -4.406713437784E+00 2.087829027681E+00 2.611791998996E+00
H 9.265462226216E+00 1.539163456778E-01 3.340179224739E+00
H 3.405958370216E+00 -1.838787148950E+00 2.792731515148E+00
H -2.453545485784E+00 -3.129136450755E+00 1.178555288224E+00
H -8.313049341784E+00 -3.224261983808E+00 -8.857890011812E-01
H 5.359126322216E+00 -2.087829027681E+00 -2.611791998996E+00
H -5.003775337840E-01 -1.539163456778E-01 -3.340179224739E+00
H -6.359881389784E+00 1.838787148950E+00 -2.792731515148E+00
H 7.312294274216E+00 3.129136450755E+00 -1.178555288224E+00
H -4.104284262858E-01 1.634948761011E+00 3.343620778082E+00
H -6.269932282286E+00 -6.426296500251E-01 3.666044802190E+00
H 7.402243381714E+00 -2.674745376930E+00 2.588164316141E+00
H 1.542739525714E+00 -3.685199281099E+00 5.216930297957E-01
H -4.316764330286E+00 -3.288032315205E+00 -1.744047262237E+00

H 9.355411333714E+00 -1.634948761011E+00 -3.343620778082E+00
H 3.495907477714E+00 6.426296500251E-01 -3.666044802190E+00
H -2.363596378286E+00 2.674745376930E+00 -2.588164316141E+00
H -8.223100234286E+00 3.685199281099E+00 -5.216930297957E-01
H 5.449075429714E+00 3.288032315205E+00 1.744047262237E+00

PbE0/POB-TZVP optimized geometry, *all*-[−73.6]-$(SnMe_2)_\infty$

Energy (a.u): -3.0772906791806E+03
Unit cell length (Å): 72.2292533600

Sn	-3.357992285936E-05	1.326082204820E+00	2.608158846869E-01
Sn	2.147352822981E+01	1.262929621035E+00	4.811732660476E-01
Sn	-2.928216332046E+01	1.163444851462E+00	6.876881686141E-01
Sn	-7.808601510734E+00	1.030489891792E+00	8.744195346402E-01
Sn	1.366496029900E+01	8.678896141427E-01	1.035995442706E+00
Sn	3.513852210873E+01	6.803217324575E-01	1.167767648118E+00
Sn	-1.561716944154E+01	4.731822331882E-01	1.265945304443E+00
Sn	5.856392368185E+00	2.524301425907E-01	1.327704019259E+00
Sn	2.732995417791E+01	2.441609638935E-02	1.351267106786E+00
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Sn	-3.123430530317E+01	-8.298964221991E-01	1.066672802722E+00
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H -1.587754773055E+01 -3.415218491413E+00 -2.088080751306E-01
H 5.596014079178E+00 -3.330804946463E+00 -7.829792876849E-01
H 2.706957588891E+01 -3.150570207585E+00 -1.334625611699E+00
H -2.368611566136E+01 -2.879699300064E+00 -1.847877186812E+00
H -2.212553851633E+00 -2.525984686735E+00 -2.307968699681E+00
H 1.926100795810E+01 -2.099602093017E+00 -2.701664155169E+00
H -3.149468359217E+01 -1.612817769819E+00 -3.017637651820E+00
H -1.002112178244E+01 -1.079635615834E+00 -3.246799207427E+00
H 1.145244002729E+01 -5.153943108683E-01 -3.382556261269E+00
H 3.292600183702E+01 6.367395004488E-02 -3.421003330079E+00
H -1.782968971325E+01 6.409104273461E-01 -3.361034361688E+00
H 3.643872096475E+00 1.199709078555E+00 -3.204374554131E+00
H 2.511743390621E+01 1.723994283879E+00 -2.955530724841E+00
H -2.563825764407E+01 2.198683312524E+00 -2.621661657719E+00
H -4.164695834336E+00 2.610120225401E+00 -2.212372157952E+00
H 1.730886597539E+01 2.946468731627E+00 -1.739436739256E+00
H -3.344682557488E+01 3.198052697065E+00 -1.216460892557E+00
H -1.197326376515E+01 3.357634509090E+00 -6.584896807832E-01
H 9.500298044583E+00 3.420623289517E+00 -8.157491980259E-02
H 3.097385985431E+01 3.385206965818E+00 4.976866030976E-01
H -1.978183169596E+01 3.252404401144E+00 1.062630588562E+00
H -1.691422507960E+00 3.405817248408E+00 -3.321659226464E-01
H 1.978213930177E+01 3.412963981178E+00 2.481978906116E-01
H -3.097355224850E+01 3.321925954177E+00 8.214215024495E-01
H -9.499990438771E+00 3.135322165690E+00 1.371014313220E+00
H 1.197357137096E+01 2.858520866962E+00 1.881165538399E+00
H 3.344713318069E+01 2.499485127388E+00 2.337199056068E+00

H -1.730855836958E+01 2.068543751501E+00 2.725995612221E+00
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H -2.511712630039E+01 4.764136118131E-01 3.388650970549E+00
H -3.643564490662E+00 -1.031239580980E-01 3.420422602397E+00
H 1.782999731907E+01 -6.796948394918E-01 3.353794903522E+00
H -3.292569423120E+01 -1.236712137871E+00 3.190684631512E+00
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H 3.149499119799E+01 -2.635747912371E+00 2.182374457364E+00
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H 2.173428128447E+01 -1.873196480358E-01 -3.416846013384E+00
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H 3.539927516339E+01 2.000789609630E+00 -2.776106314196E+00
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H -2.316498431769E+01 3.300691354357E+00 -9.029739270829E-01
H 1.456421718342E+00 1.575800118095E+00 2.573531323657E+00
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H -2.782570802220E+01 6.284406929813E-01 2.951486368160E+00
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H 1.512141559726E+01 -3.907150076509E-01 2.992248530592E+00
H -3.563427595301E+01 -8.907873842292E-01 2.883176602661E+00
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H -2.196928207409E+01 -2.504333631952E+00 1.683604034773E+00
H -4.957202643608E-01 -2.752841535445E+00 1.236152485238E+00
H 2.097784154537E+01 -2.922155200049E+00 7.531390793604E-01
H -2.977785000490E+01 -3.007403779902E+00 2.484592334062E-01
H -8.304288195172E+00 -3.006134828573E+00 -2.633683323245E-01

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H 3.464283542429E+01 -2.746678255705E+00 -1.249787200155E+00
H -1.611285612598E+01 -2.495954727374E+00 -1.696001027396E+00
H 5.360705683747E+00 -2.173427125911E+00 -2.093423992980E+00
H 2.683426749348E+01 -1.788373983184E+00 -2.430622961774E+00
H -2.392142405679E+01 -1.351872577045E+00 -2.697897333381E+00
H -2.447862247064E+00 -8.764802582132E-01 -2.887558110756E+00
H 1.902569956267E+01 -3.758731981558E-01 -2.994149098649E+00
H -3.172999198760E+01 1.355470494619E-01 -3.014603868407E+00
H -1.025643017787E+01 6.430678552566E-01 -2.948333973546E+00
H 1.121713163186E+01 1.132088769686E+00 -2.797245878285E+00
H 3.269069344159E+01 1.588541551401E+00 -2.565686112038E+00
H -1.806499810869E+01 1.999294884932E+00 -2.260316227681E+00
H 3.408563701045E+00 2.352532144730E+00 -1.889921160801E+00
H 2.488212551077E+01 2.638091337970E+00 -1.465156503095E+00
H -2.587356603950E+01 2.847757446576E+00 -9.982419603990E-01
H -4.400004229766E+00 2.975498758344E+00 -5.026098139969E-01
H 1.707355757996E+01 3.017640388311E+00 7.481501654561E-03
H -3.368213397031E+01 2.972969998510E+00 5.173575881249E-01
H -1.220857216058E+01 2.842772674725E+00 1.012350238735E+00
H 9.264989649153E+00 2.630793956912E+00 1.478219416159E+00
H 3.073855145888E+01 2.343132086832E+00 1.901562912367E+00
H -2.001714009139E+01 1.988062572744E+00 2.270201905753E+00

PbE0/POB-TZVP optimized geometry, *all*-[60.4]-$(SnMe_2)_\infty$

Energy (a.u): -1.7465688746416E+03
Unit cell length (Å): 37.0362166100

Sn	-3.938731500172E-04	1.580771827487E+00	3.110166979495E-01
Sn	-7.054911322674E+00	1.418868789451E+00	7.631397744207E-01
Sn	-1.410942877220E+01	1.130893032868E+00	1.147454532951E+00
Sn	1.587227038828E+01	7.424324674736E-01	1.429812920707E+00
Sn	8.817752938755E+00	2.880035192324E-01	1.585126155828E+00
Sn	1.763235489231E+00	-1.920158055751E-01	1.599593975792E+00
Sn	-5.291281960293E+00	-6.549736834098E-01	1.471930851304E+00
Sn	-1.234579940982E+01	-1.059734275169E+00	1.213480211216E+00
Sn	1.763589975066E+01	-1.370332826012E+00	8.472065290908E-01
Sn	1.058138230114E+01	-1.559171291657E+00	4.056548289514E-01
Sn	3.526864851612E+00	-1.609470545728E+00	-7.194108292710E-02
Sn	-3.527652597912E+00	-1.516761278766E+00	-5.431447138793E-01
Sn	-1.058217004744E+01	-1.289281115989E+00	-9.660875534521E-01
Sn	-1.763668749696E+01	-9.472426681384E-01	-1.303189274295E+00
Sn	1.234501166352E+01	-5.210375523181E-01	-1.524496909165E+00
Sn	5.290494213993E+00	-4.853596343865E-02	-1.610346303511E+00
Sn	-1.764023235531E+00	4.282782587889E-01	-1.553109361902E+00
Sn	-8.818540685055E+00	8.670380782548E-01	-1.357871837780E+00
Sn	-1.587305813458E+01	1.228757759534E+00	-1.041981441949E+00
Sn	1.410864102590E+01	1.481296921564E+00	-6.335064223397E-01
Sn	7.054123576374E+00	1.602216351548E+00	-1.687415770088E-01
C	1.140416412902E+00	3.094162642521E+00	-7.355572255736E-01
C	-5.914101036622E+00	3.173506976186E+00	2.091419674943E-01
C	-1.296861848615E+01	2.970871288310E+00	1.135257978946E+00
C	1.701308067433E+01	2.504260649014E+00	1.960501336971E+00
C	9.958563224806E+00	1.815135461287E+00	2.611545547687E+00
C	2.904045775283E+00	9.647275222333E-01	3.030542475913E+00
C	-4.150471674241E+00	2.859930919221E-02	3.180262405837E+00
C	-1.120498912377E+01	-9.100700779766E-01	3.047402064651E+00
C	-1.825950657329E+01	-1.767875744940E+00	2.643766676717E+00
C	1.172219258719E+01	-2.468597893771E+00	2.005221017577E+00
C	4.667675137664E+00	-2.949974286477E+00	1.188502671259E+00
C	-2.386842311860E+00	-3.169232518081E+00	2.661806469408E-01
C	-9.441359761384E+00	-3.106890532505E+00	-6.797926959724E-01
C	-1.649587721091E+01	-2.768487688752E+00	-1.565363474627E+00
C	1.348582194957E+01	-2.184092564544E+00	-2.311844839077E+00
C	6.431304500045E+00	-1.405631231245E+00	-2.852908644211E+00
C	-6.232129494793E-01	-5.022733945388E-01	-3.140478996523E+00
C	-7.677730399003E+00	4.457136374628E-01	-3.149004008230E+00
C	-1.473224784853E+01	1.354097056794E+00	-2.877726194628E+00

C 1.524945131195E+01 2.142163010272E+00 -2.350749779940E+00
C 8.194933862426E+00 2.739888379559E+00 -1.614898931210E+00
C -1.140434103395E+00 2.585794545323E+00 1.852882515921E+00
C -8.194951552919E+00 1.924768239718E+00 2.532740466728E+00
C -1.524946900244E+01 1.092717829307E+00 2.987553312318E+00
C 1.473223015803E+01 1.635746444492E-01 3.176908935447E+00
C 7.677712708510E+00 -7.801028654033E-01 3.083982258026E+00
C 6.231952589860E-01 -1.654464812240E+00 2.717030223146E+00
C -6.431322190538E+00 -2.381820300009E+00 2.108658129449E+00
C -1.348583964006E+01 -2.897540601677E+00 1.312922507256E+00
C 1.649585952041E+01 -3.155801705238E+00 4.005279586288E-01
C 9.441342070891E+00 -3.133655978281E+00 -5.474552568110E-01
C 2.386824621367E+00 -2.833071165831E+00 -1.446794670215E+00
C -4.667692828157E+00 -2.280755547569E+00 -2.217580028017E+00
C -1.172221027768E+01 -1.525784789975E+00 -2.791323668640E+00
C 1.825948888280E+01 -6.352413579945E-01 -3.117045951782E+00
C 1.120497143327E+01 3.117460563541E-01 -3.165805023177E+00
C 4.150453983748E+00 1.231033465521E+00 -2.933268425357E+00
C -2.904063465776E+00 2.040938148974E+00 -2.440098055507E+00
C -9.958580915300E+00 2.669496521382E+00 -1.730114265231E+00
C -1.701309836482E+01 3.060858412972E+00 -8.664022300085E-01
C 1.296860079565E+01 3.180249602214E+00 7.429344549415E-02
C 5.914083346129E+00 3.017061658004E+00 1.008387822333E+00
H 4.966987487346E-01 3.924086411289E+00 -1.022990951025E+00
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H -1.361233615031E+01 3.818503668703E+00 1.365281795543E+00
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H 2.260328111116E+00 1.313377805601E+00 3.836665660296E+00
H -4.794189338408E+00 1.241510588984E-01 4.053338274030E+00
H -1.184870678793E+01 -1.076107054215E+00 3.909853994334E+00
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H -5.468544489075E+00 3.043890396177E+00 -7.752817626948E-01
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H -3.704915126694E+00 1.000584131818E+00 2.977442182589E+00
H -1.075943257622E+01 7.851449643861E-02 3.140090130770E+00
H -1.781395002574E+01 -8.505314965042E-01 3.023727290772E+00
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H 1.605105190635E+01 -3.086813348429E+00 -5.903201480981E-01
H 8.996534456829E+00 -2.775674974086E+00 -1.473948087120E+00
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H -5.112500442219E+00 -1.463065766469E+00 -2.781426448475E+00
H -1.216701789174E+01 -5.782260215827E-01 -3.089101680627E+00
H 1.781468126873E+01 3.579916428241E-01 -3.122296672156E+00
H 1.076016381921E+01 1.262400178745E+00 -2.878061902391E+00
H 3.705646369686E+00 2.054638918833E+00 -2.378098702431E+00
H -3.348871079838E+00 2.664313974348E+00 -1.666830996647E+00
H -1.040338852936E+01 3.037253041093E+00 -8.074580420425E-01
H -1.745790597889E+01 3.140318846372E+00 1.236611030685E-01
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H 5.469275732067E+00 2.524992414827E+00 1.871178193106E+00
H -1.938500740791E+00 3.184639808237E+00 1.415929632131E+00
H -8.993018190315E+00 2.625802611303E+00 2.291712913484E+00
H -1.604753563984E+01 1.833651329210E+00 2.963867445457E+00
H 1.393416352064E+01 8.785720796697E-01 3.372669348184E+00

H 6.879646071114E+00 -1.545721546989E-01 3.481794778609E+00
H -1.748713784101E-01 -1.173981974794E+00 3.281547463349E+00
H -7.229388827934E+00 -2.089078344493E+00 2.789720255137E+00
H -1.428390627746E+01 -2.818550935515E+00 2.050014159771E+00
H 1.569779288302E+01 -3.297582906909E+00 1.128155309970E+00
H 8.643275433495E+00 -3.483610165821E+00 1.060549100499E-01
H 1.588757983971E+00 -3.360103373927E+00 -9.254689340422E-01
H -5.465759465553E+00 -2.938036651690E+00 -1.874760801991E+00
H -1.252027691508E+01 -2.254912479588E+00 -2.657471945431E+00
H 1.746142224540E+01 -1.371429438154E+00 -3.204055044396E+00
H 1.040690479588E+01 -3.660888727219E-01 -3.465943791902E+00
H 3.352387346352E+00 6.717802956065E-01 -3.419868223454E+00
H -3.702130103172E+00 1.649958836611E+00 -3.069922355507E+00
H -1.075664755270E+01 2.481531294257E+00 -2.447200414142E+00
H -1.781116500222E+01 3.092608806389E+00 -1.607033976617E+00
H 1.217053415826E+01 3.428894454382E+00 -6.240755179182E-01
H 5.116016708733E+00 3.460507782648E+00 4.143347892584E-01
H 1.937956953786E+00 3.483381320250E+00 -1.039865206492E-01
H -5.116560495738E+00 3.359275026845E+00 9.273779772893E-01
H -1.217107794526E+01 2.936682405369E+00 1.876340872214E+00
H 1.781062121521E+01 2.253152664757E+00 2.658582646457E+00
H 1.075610376569E+01 1.369420422084E+00 3.204597685564E+00
H 3.701586316167E+00 3.640091653065E-01 3.465870157163E+00
H -3.352931133357E+00 -6.737459032364E-01 3.419184855578E+00
H -1.040744858288E+01 -1.651635691592E+00 3.068689974729E+00
H -1.746196603240E+01 -2.482770400665E+00 2.445528522901E+00
H 1.251973312807E+01 -3.093300064181E+00 1.605071129789E+00
H 5.465215678548E+00 -3.428976442271E+00 6.219961230556E-01
H -1.589301770976E+00 -3.459973215649E+00 -4.163459687960E-01
H -8.643819220500E+00 -3.183536184975E+00 -1.417693894216E+00
H -1.569833667002E+01 -2.624227993548E+00 -2.293073495688E+00
H 1.428336249045E+01 -1.831745628658E+00 -2.964703454080E+00
H 7.228845040929E+00 -8.765046261796E-01 -3.372906500191E+00
H 1.743275914050E-01 1.566176588124E-01 -3.481412002003E+00
H -6.880189858119E+00 1.175823777514E+00 -3.280578769513E+00
H -1.393470730764E+01 2.090552793565E+00 -2.788251716768E+00
H 1.604699185283E+01 2.819527019669E+00 -2.048176262948E+00
H 8.992474403310E+00 3.297973896784E+00 -1.126111359891E+00
H -4.964746410783E-01 3.245719028055E+00 2.432176681208E+00
H -7.550992090602E+00 2.384624176564E+00 3.280814373633E+00
H -1.460550954013E+01 1.311645002235E+00 3.837937311343E+00
H 1.537618962035E+01 1.221204133981E-01 4.054042676431E+00
H 8.321672170826E+00 -1.078255110086E+00 3.909928558844E+00
H 1.267154721303E+00 -2.182822935194E+00 3.418400130365E+00
H -5.787362728221E+00 -3.093437363350E+00 2.623131848901E+00

H -1.284188017774E+01 -3.729186306446E+00 1.594786791238E+00
H 1.713981898273E+01 -4.033580680949E+00 4.247379285670E-01
H 1.008530153321E+01 -3.979573710873E+00 -7.830507629891E-01
H 3.030784083684E+00 -3.571964152514E+00 -1.921261957892E+00
H -4.023733365840E+00 -2.846969903898E+00 -2.888760596517E+00
H -1.107825081536E+01 -1.869009885599E+00 -3.599580179024E+00
H -1.813276826489E+01 -7.249801369496E-01 -3.990561266128E+00
H 1.184893089559E+01 4.834672783908E-01 -4.026963472446E+00
H 4.794413446065E+00 1.648956504385E+00 -3.705552302200E+00
H -2.260104003459E+00 2.667928708638E+00 -3.054886548354E+00
H -9.314621452983E+00 3.449843739116E+00 -2.132780718539E+00
H -1.636913890251E+01 3.925225013984E+00 -1.021167962327E+00
H 1.361256025797E+01 4.051832820793E+00 1.811800486591E-01
H 6.558042808446E+00 3.818417500300E+00 1.367429417226E+00

PbE0/POB-TZVP optimized geometry, *all*-[43.4]-$(SnMe_2)_\infty$

Energy (a.u): -4.1584886952393E+02
Unit cell length (Å): 7.70401244000

Sn	3.849399191590E-04	1.963788313102E+00	3.858946526302E-01
Sn	1.541187427919E+00	2.398363381160E-01	1.986921677501E+00
Sn	3.081989915919E+00	-1.815561304409E+00	8.420904770494E-01
Sn	-3.081220036081E+00	-1.361914932900E+00	-1.466481141082E+00
Sn	-1.540417548081E+00	9.738515860908E-01	-1.748425666099E+00
C	1.317042802934E+00	3.449399242110E+00	-4.798701983185E-01
C	2.857845290934E+00	1.522306665283E+00	3.132285580138E+00
C	-3.305364661066E+00	-2.508561981665E+00	2.415729149315E+00
C	-1.764562173066E+00	-3.072683232837E+00	-1.639282858247E+00
C	-2.237596850660E-01	6.095393071094E-01	-3.428861672887E+00
C	-1.317031160459E+00	3.010283147761E+00	1.749538461995E+00
C	2.237713275406E-01	-7.336813042507E-01	3.403586520641E+00
C	1.764573815541E+00	-3.463723130698E+00	3.539936914119E-01
C	3.305376303541E+00	-1.407017318140E+00	-3.184806387545E+00
C	-2.857833648459E+00	2.594138605328E+00	-2.322312286503E+00
H	7.407104460519E-01	4.284826534464E+00	-8.745966442733E-01
H	2.281512934052E+00	2.155875054764E+00	3.804846970493E+00
H	3.822315422052E+00	-2.952422475122E+00	3.226121394030E+00
H	-2.340894529948E+00	-3.980572493538E+00	-1.810994297149E+00
H	-8.000920419481E-01	4.922933794321E-01	-4.345377423100E+00
H	1.900429794250E+00	3.022345650567E+00	-1.293236294701E+00
H	3.441232282250E+00	2.163896974085E+00	2.474789532663E+00
H	-2.721977669750E+00	-1.684983772429E+00	2.822740340889E+00
H	-1.181175181750E+00	-3.205274215939E+00	-7.302400605780E-01
H	3.596273062502E-01	-2.959846362844E-01	-3.274053518273E+00
H	-1.899387880898E+00	2.306686670127E+00	2.341221770285E+00
H	-3.585853928980E-01	-1.513828838954E+00	2.917266703294E+00
H	1.182217095102E+00	-3.242284345751E+00	-5.382517934009E-01
H	2.723019583102E+00	-4.900130879113E-01	-3.249924606121E+00
H	-3.440190368898E+00	2.939439602489E+00	-1.470312074057E+00
H	-2.004913535991E+00	3.651369512173E+00	1.199478814532E+00
H	-4.641110479908E-01	-1.243691071463E-02	3.843318106037E+00
H	1.076691440009E+00	-3.659055945710E+00	1.175822404577E+00
H	2.617493928009E+00	-2.248984030471E+00	-3.116619895275E+00
H	-3.545716023991E+00	2.269107374723E+00	-3.101999429870E+00
H	2.003984039491E+00	3.835569494334E+00	2.722640397622E-01
H	3.544786527491E+00	9.263176676866E-01	3.731977576533E+00
H	-2.618423424509E+00	-3.263073691324E+00	2.034224947788E+00
H	-1.077620936509E+00	-2.943008116721E+00	-2.474757418037E+00
H	4.631815514910E-01	1.444194646024E+00	-3.563709146046E+00

H -7.412194452980E-01 3.635087639641E+00 2.430685271157E+00
H 7.995830427020E-01 -1.188415209505E+00 4.208296843749E+00
H 2.340385530702E+00 -4.369568631862E+00 1.701852130287E-01
H -3.822824421298E+00 -1.512126721161E+00 -4.103116597715E+00
H -2.282021933298E+00 3.435022922888E+00 -2.706050730220E+00

PbE0/POB-TZVP optimized geometry, *all*-[24.5]-$(SnMe_2)_\infty$

Energy (a.u): -1.0811897749962E+03
Unit cell length (Å): 15.1479959700

Sn	-5.669095694053E-04	2.700825898701E+00	5.318428274484E-01
Sn	-6.991949664954E+00	2.144302880444E+00	1.726059815047E+00
Sn	1.164663549661E+00	1.096545913929E+00	2.524857300294E+00
Sn	-5.826719205723E+00	-2.024165066564E-01	2.745240405873E+00
Sn	2.329894008892E+00	-1.455007744950E+00	2.336722018199E+00
Sn	-4.661488746492E+00	-2.374274243620E+00	1.392888776709E+00
Sn	3.495124468123E+00	-2.749623126183E+00	1.299615026049E-01
Sn	-3.496258287262E+00	-2.495066487089E+00	-1.162738385540E+00
Sn	4.660354927354E+00	-1.668920184613E+00	-2.189068922075E+00
Sn	-2.331027828031E+00	-4.604443805104E-01	-2.713910149703E+00
Sn	5.825585386584E+00	8.535136822104E-01	-2.617027268196E+00
Sn	-1.165797368800E+00	1.971942046292E+00	-1.920614978143E+00
Sn	6.990815845815E+00	2.638622252046E+00	-7.842129425177E-01
C	1.519247774003E+00	4.134237131427E+00	-4.370974977277E-02
C	-5.472134981382E+00	3.680998113065E+00	1.882572732382E+00
C	2.684478233234E+00	2.384486787836E+00	3.377580489009E+00
C	-4.306904522151E+00	5.417182756945E-01	4.098825259861E+00
C	3.849708692464E+00	-1.425151364995E+00	3.881078559878E+00
C	-3.141674062920E+00	-3.065536002901E+00	2.774223533894E+00
C	5.014939151695E+00	-4.003643286255E+00	1.031827329313E+00
C	-1.976443603689E+00	-4.024564141861E+00	-9.469480815461E-01
C	6.180169610926E+00	-3.123505853822E+00	-2.708789098885E+00
C	-8.112131444587E-01	-1.506890016998E+00	-3.850079178117E+00
C	7.345400070157E+00	4.549361627265E-01	-4.109362516126E+00
C	3.540173147721E-01	2.312541950145E+00	-3.427240424877E+00
C	-6.637365440613E+00	3.640372245938E+00	-1.959978855014E+00
C	-1.519269518297E+00	3.810286626619E+00	1.608120501838E+00
C	6.637343696319E+00	2.626510392363E+00	3.194648475847E+00
C	-3.540390590659E-01	8.410322800979E-01	4.049320983728E+00
C	-7.345421814450E+00	-1.137116192000E+00	3.976342853844E+00
C	8.111914001649E-01	-2.854765048246E+00	2.992432496271E+00
C	-6.180191355220E+00	-3.918421635587E+00	1.322991916523E+00
C	1.976421859396E+00	-4.084415048315E+00	-6.495301675194E-01
C	-5.014960895989E+00	-3.314718196012E+00	-2.473252717870E+00
C	3.141652318626E+00	-1.785659351687E+00	-3.730382876483E+00
C	-3.849730436758E+00	1.524725305820E-01	-4.132927274081E+00
C	4.306882777857E+00	2.055674793588E+00	-3.588667840360E+00
C	-2.684499977527E+00	3.487946734949E+00	-2.222287852548E+00
C	5.472113237088E+00	4.121172113648E+00	-3.468084991894E-01
H	1.076893689146E+00	4.957994945402E+00	-6.023045994028E-01

H -5.914489066238E+00 4.669991403535E+00 1.770780901184E+00
H 2.242124148377E+00 3.312149110616E+00 3.738201837533E+00
H -4.749258607008E+00 1.195533372179E+00 4.849245783119E+00
H 3.407354607608E+00 -1.194964654086E+00 4.849385959539E+00
H -3.584028147777E+00 -3.311710678985E+00 3.738590254065E+00
H 4.572585066839E+00 -4.669783697768E+00 1.771328576281E+00
H -2.418797688546E+00 -4.958065548387E+00 -6.017231315050E-01
H 5.737815526069E+00 -4.110514333038E+00 -2.836927321414E+00
H -1.253567229315E+00 -2.321293821057E+00 -4.422225650667E+00
H 6.903045985300E+00 -2.928692958076E-04 -4.994445376948E+00
H -8.833677008455E-02 2.320775175292E+00 -4.422497856963E+00
H -7.079719525469E+00 4.110181595593E+00 -2.837409374824E+00
H 2.277340656454E+00 3.665539593225E+00 -6.680577622026E-01
H -4.714042098931E+00 3.556136042451E+00 1.111925415989E+00
H 3.442571115685E+00 2.632064580436E+00 2.637179881531E+00
H -3.548811639700E+00 1.105018842860E+00 3.558288217678E+00
H 4.607801574915E+00 -6.751733946940E-01 3.664235605176E+00
H -2.383581180469E+00 -2.300691544245E+00 2.930750774354E+00
H 5.773032034146E+00 -3.399148987349E+00 1.525866260504E+00
H -1.218350721239E+00 -3.718902361637E+00 -2.285758249464E-01
H 6.938262493377E+00 -3.186700022506E+00 -1.930653943538E+00
H -5.312026200776E-02 -1.924463112117E+00 -3.190442510568E+00
H -7.044503017392E+00 -2.213548950368E-01 -3.719339147427E+00
H 1.112110197223E+00 1.532463060881E+00 -3.396180008506E+00
H -5.879272558162E+00 2.935212197732E+00 -2.294996958042E+00
H -2.276439269146E+00 3.140311442734E+00 2.010627649226E+00
H 5.880173945470E+00 1.846222430449E+00 3.239697862225E+00
H -1.111208809915E+00 1.291861087410E-01 3.726592337580E+00
H 7.045404404700E+00 -1.617445193619E+00 3.359769418701E+00
H 5.402164931570E-02 -2.993539294448E+00 2.223263815609E+00
H -6.937361106069E+00 -3.683849618978E+00 5.774352655941E-01
H 1.219252108546E+00 -3.530234391001E+00 -1.200676744919E+00
H -5.772130646838E+00 -2.567885007983E+00 -2.703728182894E+00
H 2.384482567777E+00 -1.017264116004E+00 -3.587388077625E+00
H -4.606900187607E+00 7.663997255896E-01 -3.649220596486E+00
H 3.549713027008E+00 2.374490626169E+00 -2.875060654566E+00
H -3.441669728377E+00 3.438614340006E+00 -1.442258964923E+00
H 4.714943486239E+00 3.714992948344E+00 3.209468724794E-01
H -2.010110186934E+00 4.523795355980E+00 9.476905443828E-01
H 6.146503027681E+00 3.565208100873E+00 2.941450830486E+00
H -8.448797277033E-01 1.789874635271E+00 4.261360179651E+00
H 7.311733486912E+00 -3.954975389433E-01 4.605043266614E+00
H 3.203507315275E-01 -2.490265993248E+00 3.893766437984E+00
H -6.671032023857E+00 -4.014544519458E+00 2.290474643384E+00
H 1.485581190758E+00 -4.619139276767E+00 1.624627111968E-01

H -5.505801564626E+00 -4.165544892431E+00 -2.002767470238E+00
H 2.650811649989E+00 -2.757674373497E+00 -3.709187760205E+00
H -4.340571105396E+00 -7.180538891735E-01 -4.565877834868E+00
H 3.816042109220E+00 1.486064087672E+00 -4.376580322356E+00
H -3.175340646165E+00 3.349742691045E+00 -3.184661001502E+00
H 4.981272568451E+00 4.446035612676E+00 -1.263174224530E+00
H 2.008707395078E+00 4.545605760464E+00 8.379957614643E-01
H -4.982675360307E+00 3.635497962420E+00 2.854456724324E+00
H 3.173937854308E+00 1.892541393685E+00 4.216996051573E+00
H -3.817444901076E+00 -2.839736007464E-01 4.613472403719E+00
H 4.339168313539E+00 -2.395433665500E+00 3.953057826542E+00
H -2.652214441846E+00 -3.958128745593E+00 2.387045340816E+00
H 5.504398772770E+00 -4.614064230692E+00 2.741895345233E-01
H -1.486983982615E+00 -4.212973206042E+00 -1.901479789786E+00
H 6.669629232001E+00 -2.846740791719E+00 -3.641543009571E+00
H -3.217535233840E-01 -8.283543689586E-01 -4.547372611214E+00
H -7.313136278769E+00 1.379798056978E+00 -4.411453949409E+00
H 8.434769358468E-01 3.271855376430E+00 -3.264924351577E+00
H -6.147905819538E+00 4.414370059274E+00 -1.370439931403E+00
H -1.075803630734E+00 4.362495585107E+00 2.435581388880E+00
H 7.080809583882E+00 2.730926893907E+00 4.183953003090E+00
H 8.942682849725E-02 4.737357625505E-01 4.97383406393E+00
H -6.901955926887E+00 -1.891982522872E+00 4.624264975657E+00
H 1.254657287728E+00 -3.824270413166E+00 3.215335167432E+00
H -5.736725467657E+00 -4.880464039257E+00 1.069810821338E+00
H 2.419887746959E+00 -4.818602169923E+00 -1.320794291307E+00
H -4.571495008426E+00 -3.652856613911E+00 -3.408821349110E+00
H 3.585118206190E+00 -1.650285629346E+00 -4.715928516582E+00
H -3.406264549195E+00 7.303459048047E-01 -4.942673294005E+00
H 4.750348665420E+00 2.943663993787E+00 -4.037111185442E+00
H -2.241034089964E+00 4.482624136789E+00 -2.206695556758E+00
H 5.915579124651E+00 4.994669111530E+00 1.292474304147E-01

PbE0/POB-TZVP optimized geometry, *all*-[180]-$(PbMe_2)_\infty$

Energy (a.u): -5.4521279746303E+02
Unit cell length (Å): 4.89520208

Pb	-1.626066520348E+00	7.877438116441E-01	-1.433274007202E-01
Pb	8.215345196516E-01	-7.877438116441E-01	1.433274007202E-01
C	-1.616491536716E+00	1.834157669003E+00	-2.134081246705E+00
C	8.311095032844E-01	-1.834157669003E+00	2.134081246705E+00
C	-1.615866382059E+00	2.468217324483E+00	1.351451076200E+00
C	8.317346579409E-01	-2.468217324483E+00	-1.351451076200E+00
H	-1.615595548314E+00	1.114218304703E+00	-2.949095469426E+00
H	8.320054916858E-01	-1.114218304703E+00	2.949095469426E+00
H	-7.289499738392E-01	2.459595746420E+00	-2.214775483536E+00
H	1.718651066161E+00	-2.459595746420E+00	2.214775483536E+00
H	2.395028169268E+00	2.464239088864E+00	-2.220955572775E+00
H	-5.257287073157E-02	-2.464239088864E+00	2.220955572775E+00
H	-7.285266303481E-01	3.082173006560E+00	1.206182604995E+00
H	1.719074409652E+00	-3.082173006560E+00	-1.206182604995E+00
H	-1.614185220861E+00	2.081337185187E+00	2.367746664302E+00
H	8.334158191385E-01	-2.081337185187E+00	-2.367746664302E+00
H	2.395454342706E+00	3.088405347166E+00	1.211587056480E+00
H	-5.214669729434E-02	-3.088405347166E+00	-1.211587056480E+00

PbE0/POB-TZVP optimized geometry, *all*-[-170.6]-$(PbMe_2)_\infty$

Energy (a.u): -6.2699481644440E+03
Unit cell length (Å): 56.04125950

Pb	-2.346947788562E+00	7.688802375087E-01	-2.580413441580E-01
Pb	-7.220100788562E+00	8.099867940761E-01	-4.103106565391E-02
Pb	-1.209325378856E+01	7.910203355698E-01	1.790222992851E-01
Pb	-1.696640678856E+01	7.133875174516E-01	3.857983992587E-01
Pb	-2.183955978856E+01	5.828460106947E-01	5.639615968694E-01
Pb	-2.671271278856E+01	4.090774816677E-01	7.002983427930E-01
Pb	2.445539371144E+01	2.049695472304E-01	7.846971642834E-01
Pb	1.958224071144E+01	-1.434004085175E-02	8.108985868496E-01
Pb	1.470908771144E+01	-2.325860937052E-01	7.769593708433E-01
Pb	9.835934711438E+00	-4.335822999992E-01	6.853966326542E-01
Pb	4.962781711438E+00	-6.024216906092E-01	5.430011617021E-01
Pb	8.962871143789E-02	-7.265822203227E-01	3.603337786515E-01
Pb	-4.783524288562E+00	-7.968554706472E-01	1.509420876558E-01
Pb	-9.656677288562E+00	-8.080295960851E-01	-6.964428746733E-02
Pb	-1.452983028856E+01	-7.592758628708E-01	-2.850654643904E-01
Pb	-1.940298328856E+01	-6.542101123633E-01	-4.793446399073E-01
Pb	-2.427613628856E+01	-5.006245906339E-01	-6.380730163382E-01
Pb	2.689197021144E+01	-3.099100332224E-01	-7.494784361370E-01
Pb	2.201881721144E+01	-9.621086639077E-02	-8.052984689633E-01
Pb	1.714566421144E+01	1.246238202656E-01	-8.013931983419E-01
Pb	1.227251121144E+01	3.362157282889E-01	-7.380522603295E-01
Pb	7.399358211438E+00	5.228720538297E-01	-6.199733625328E-01
Pb	2.526205211438E+00	6.707493511184E-01	-4.559138766265E-01
C	-2.133573180449E+00	1.523051920654E+00	-2.366251666015E+00
C	-7.006726180449E+00	2.104980083162E+00	-1.867590144924E+00
C	-1.187987918045E+01	2.530791502545E+00	-1.230418006441E+00
C	-1.675303218045E+01	2.768905693784E+00	-5.019913932081E-01
C	-2.162618518045E+01	2.801662816617E+00	2.636656252014E-01
C	-2.649933818045E+01	2.626633425095E+00	1.009767770380E+00
C	2.466876831955E+01	2.256798648483E+00	1.680980059409E+00
C	1.979561531955E+01	1.719587440280E+00	2.227521747404E+00
C	1.492246231955E+01	1.054842298220E+00	2.608858337628E+00
C	1.004930931955E+01	3.118643284831E-01	2.796707839683E+00
C	5.176156319551E+00	-4.542431918126E-01	2.777138315356E+00
C	3.030033195514E-01	-1.186661572596E+00	2.551601146741E+00
C	-4.570149680449E+00	-1.831070693155E+00	2.136823393871E+00
C	-9.443302680449E+00	-2.339677676994E+00	1.563567225194E+00
C	-1.431645568045E+01	-2.674761470844E+00	8.743484282686E-01
C	-1.918960868045E+01	-2.811470442620E+00	1.202832082963E-01
C	-2.406276168045E+01	-2.739665513289E+00	-6.427028669762E-01

C 2.710534481955E+01 -2.464672125973E+00 -1.358022610775E+00
C 2.223219181955E+01 -2.006885282199E+00 -1.972624030073E+00
C 1.735903881955E+01 -1.400256937933E+00 -2.440924949215E+00
C 1.248588581955E+01 -6.897779423292E-01 -2.728193631362E+00
C 7.612732819552E+00 7.185872773258E-02 -2.813124672526E+00
C 2.739579819551E+00 8.281659646902E-01 -2.689419125918E+00
C -2.310343638135E+00 2.642664664719E+00 9.857710599627E-01
C -7.183496638135E+00 2.278709641243E+00 1.662198388797E+00
C -1.205664963813E+01 1.745753148079E+00 2.215348067186E+00
C -1.692980263813E+01 1.083322130212E+00 2.604195513975E+00
C -2.180295563813E+01 3.405460658150E-01 2.799901692894E+00
C -2.667610863813E+01 -4.274867423884E-01 2.787951971949E+00
C 2.449199786187E+01 -1.163814814531E+00 2.569232607277E+00
C 1.961884486187E+01 -1.813828065978E+00 2.159965013579E+00
C 1.474569186187E+01 -2.329317987482E+00 1.590502696007E+00
C 9.872538861866E+00 -2.672053049776E+00 9.030800695379E-01
C 4.999385861865E+00 -2.816614161197E+00 1.486801256274E-01
C 1.262328618655E-01 -2.752279885435E+00 -6.167467430345E-01
C -4.746920138135E+00 -2.483821601413E+00 -1.336432327194E+00
C -9.620073138135E+00 -2.031149631941E+00 -1.957000839417E+00
C -1.449322613813E+01 -1.427836586160E+00 -2.432427552063E+00
C -1.936637913813E+01 -7.186274327012E-01 -2.727452240789E+00
C -2.423953213813E+01 4.387902993943E-02 -2.820194274079E+00
C 2.692857436187E+01 8.031311856627E-01 -2.703775399590E+00
C 2.205542136187E+01 1.502818775426E+00 -2.386829872664E+00
C 1.718226836187E+01 2.091049171554E+00 -1.892864093102E+00
C 1.230911536187E+01 2.524196016542E+00 -1.258513243032E+00
C 7.435962361865E+00 2.770134790411E+00 -5.308242230413E-01
C 2.562809361866E+00 2.810625339399E+00 2.362336012133E-01
H -2.014595857909E+00 6.963768818973E-01 -3.062799799921E+00
H -6.887748857909E+00 1.496886834807E+00 -2.761342640785E+00
H -1.176090185791E+01 2.186379538981E+00 -2.255089330284E+00
H -1.663405485791E+01 2.713718474770E+00 -1.581586360503E+00
H -2.150720785791E+01 3.039793325721E+00 -7.907843656399E-01
H -2.638036085791E+01 3.140420611832E+00 5.866648802515E-02
H 2.478774564209E+01 3.008137267632E+00 9.037663166547E-01
H 1.991459264209E+01 2.652754143604E+00 1.681837932034E+00
H 1.504143964209E+01 2.100628380288E+00 2.335175321890E+00
H 1.016828664209E+01 1.392708619741E+00 2.815323440839E+00
H 5.295133642091E+00 5.814980320860E-01 3.086671899428E+00
H 4.219806420907E-01 -2.728396044324E-01 3.129096023821E+00
H -4.451172357909E+00 -1.106941975648E+00 2.939449410789E+00
H -9.324325357909E+00 -1.858947524453E+00 2.531797282045E+00
H -1.419747835791E+01 -2.473083439488E+00 1.936373331093E+00
H -1.907063135791E+01 -2.903802069420E+00 1.197337428493E+00

H -2.394378435791E+01 -3.119158983874E+00 3.695004862761E-01
H 2.722432214209E+01 -3.103182145696E+00 -4.857406166558E-01
H 2.235116914209E+01 -2.857056483886E+00 -1.304956560166E+00
H 1.747801614209E+01 -2.399036012830E+00 -2.027389845387E+00
H 1.260486314209E+01 -1.763090015562E+00 -2.599460900468E+00
H 7.731710142091E+00 -9.963836974401E-01 -2.978741832303E+00
H 2.858557142091E+00 -1.557801586308E-01 -3.137103109274E+00
H -1.261343588989E+00 2.171265068810E+00 -2.433237180302E+00
H -6.134496588989E+00 2.747228204876E+00 -1.757205840239E+00
H -1.100764958899E+01 3.119441992720E+00 -9.508505816878E-01
H -1.588080258899E+01 3.260301038461E+00 -7.397508534446E-02
H -2.075395558899E+01 3.159358471064E+00 8.083868046653E-01
H -2.562710858899E+01 2.824100738971E+00 1.630794343497E+00
H 2.554099791101E+01 2.279392374471E+00 2.332253326259E+00
H 2.066784491101E+01 1.565631905082E+00 2.860739749161E+00
H 1.579469191101E+01 7.357556795822E-01 3.177058191881E+00
H 1.092153891101E+01 -1.486881788135E-01 3.257748762584E+00
H 6.048385911011E+00 -1.022104515190E+00 3.096827010775E+00
H 1.175232911011E+00 -1.819716035492E+00 2.706227766618E+00
H -3.697920088989E+00 -2.482367542088E+00 2.114919989179E+00
H -8.571073088989E+00 -2.960913204163E+00 1.366758271257E+00
H -1.344422608899E+01 -3.219861479163E+00 5.172303448598E-01
H -1.831737908899E+01 -3.240007358138E+00 -3.706581900446E-01
H -2.319053208899E+01 -3.019856713409E+00 -1.231056702642E+00
H 2.797757441101E+01 -2.575737111171E+00 -2.000153371314E+00
H 2.310442141101E+01 -1.940586870610E+00 -2.620907814528E+00
H 1.823126841101E+01 -1.161512179451E+00 -3.047281514994E+00
H 1.335811541101E+01 -2.962934435063E-01 -3.247652285879E+00
H 8.484962411011E+00 5.909000216908E-01 -3.207159543740E+00
H 3.611809411011E+00 1.434269135467E+00 -2.928806450021E+00
H -3.018479755902E+00 2.093231746639E+00 -2.644450816296E+00
H -7.891632755902E+00 2.729073326984E+00 -1.981640240026E+00
H -1.276478575590E+01 3.162512023347E+00 -1.171860472554E+00
H -1.763793875590E+01 3.361401670467E+00 -2.751691747375E-01
H -2.251109175590E+01 3.310991533079E+00 6.419301619540E-01
H -2.738424475590E+01 3.015020300460E+00 1.511420475168E+00
H 2.378386174410E+01 2.495438804957E+00 2.268815646028E+00
H 1.891070874410E+01 1.790782029162E+00 2.857943139563E+00
H 1.403755574410E+01 9.533111425479E-01 3.235110064656E+00
H 9.164402744098E+00 4.513752959879E-02 3.372343675898E+00
H 4.291249744098E+00 -8.663837274302E-01 3.259465984144E+00
H -5.819032559015E-01 -1.713649266837E+00 2.904848611410E+00
H -5.455056255902E+00 -2.433821279547E+00 2.334791905967E+00
H -1.032820925590E+01 -2.973487901944E+00 1.591574365820E+00
H -1.520136225590E+01 -3.292624529456E+00 7.303170359289E-01

H -2.007451525590E+01 -3.367562258374E+00 -1.851045675392E-01
H -2.494766825590E+01 -3.192743300159E+00 -1.086797812030E+00
H 2.622043824410E+01 -2.781133177201E+00 -1.907888234572E+00
H 2.134728524410E+01 -2.163259129328E+00 -2.587479314763E+00
H 1.647413224410E+01 -1.384946048084E+00 -3.075168891109E+00
H 1.160097924410E+01 -5.039178541602E-01 -3.334787258762E+00
H 6.727826244098E+00 4.144836217356E-01 -3.347079711070E+00
H 1.854673244099E+00 1.302144743544E+00 -3.111134573079E+00
H -3.141097578333E+00 3.286092835035E+00 7.000572412199E-01
H -8.014250578333E+00 2.975362415379E+00 1.560674456318E+00
H -1.288740357833E+01 2.443962976751E+00 2.305543586602E+00
H -1.776055657833E+01 1.731305984525E+00 2.879421096228E+00
H -2.263370957833E+01 8.902459476238E-01 3.239745115621E+00
H -2.750686257833E+01 -1.683955860814E-02 3.359792060637E+00
H 2.366124392167E+01 -9.226761518139E-01 3.230658598541E+00
H 1.878809092167E+01 -1.760082075802E+00 2.861921967471E+00
H 1.391493792167E+01 -2.466950764068E+00 2.280929676495E+00
H 9.041784921667E+00 -2.990856999712E+00 1.530771265973E+00
H 4.168631921667E+00 -3.292945053947E+00 6.670825534662E-01
H -7.045210783334E-01 -3.350810437752E+00 -2.460806203316E-01
H -5.577674078333E+00 -3.160161540327E+00 -1.140993120263E+00
H -1.045082707833E+01 -2.735137918233E+00 -1.951283380161E+00
H -1.532398007833E+01 -2.107261629168E+00 -2.616855878280E+00
H -2.019713307833E+01 -1.323099385147E+00 -3.088348147226E+00
H -2.507028607833E+01 -4.408089125066E-01 -3.330791762345E+00
H 2.609782042167E+01 4.741743406076E-01 -3.326205789809E+00
H 2.122466742167E+01 1.353990252082E+00 -3.074930350222E+00
H 1.635151442167E+01 2.133386900653E+00 -2.595601393430E+00
H 1.147836142167E+01 2.754560002398E+00 -1.923768555373E+00
H 6.605208421667E+00 3.171439990039E+00 -1.109258604219E+00
H 1.732055421667E+00 3.353108781991E+00 -2.124800169110E-01
H -1.376917123254E+00 3.177035693316E+00 8.170336284936E-01
H -6.250070123254E+00 2.838789556721E+00 1.643889777128E+00
H -1.112322312325E+01 2.290003385302E+00 2.348826141289E+00
H -1.599637612325E+01 1.571378138863E+00 2.879560815714E+00
H -2.086952912325E+01 7.362109644415E-01 3.196731637553E+00
H -2.574268212325E+01 -1.535576092715E-01 3.276815497908E+00
H 2.542542437675E+01 -1.031937517584E+00 3.113872943216E+00
H 2.055227137675E+01 -1.833783341018E+00 2.719988677348E+00
H 1.567911837675E+01 -2.499625843048E+00 2.124375294400E+00
H 1.080596537675E+01 -2.980082531327E+00 1.371206714238E+00
H 5.932812376746E+00 -3.239520131229E+00 5.163420049332E-01
H 1.059659376746E+00 -3.258697342815E+00 -3.768174287697E-01
H -3.813493623254E+00 -3.036191880033E+00 -1.242030037606E+00
H -8.686646623254E+00 -2.588505955163E+00 -2.015126960462E+00

H -1.355979962325E+01 -1.948842385225E+00 -2.638771135253E+00
H -1.843295262325E+01 -1.164642090936E+00 -3.066709726517E+00
H -2.330610562325E+01 -2.940656206446E-01 -3.267204486629E+00
H 2.786200087675E+01 5.983203514689E-01 -3.225385636433E+00
H 2.298884787675E+01 1.446331640247E+00 -2.944354688741E+00
H 1.811569487675E+01 2.187075127796E+00 -2.444954423311E+00
H 1.324254187675E+01 2.765613258318E+00 -1.764223073227E+00
H 8.369388876746E+00 3.139038505310E+00 -9.526473685847E-01
H 3.496235876747E+00 3.279655626509E+00 -7.041816668629E-02
H -2.395463295777E+00 2.406397714943E+00 2.043894455312E+00
H -7.268616295777E+00 1.765725835324E+00 2.617339638146E+00
H -1.214176929578E+01 9.940981481571E-01 2.996668713550E+00
H -1.701492229578E+01 1.487427490379E-01 3.153748579317E+00
H -2.188807529578E+01 -7.076442193247E-01 3.076929340397E+00
H -2.676122829578E+01 -1.511548453197E+00 2.771908328314E+00
H 2.440687820422E+01 -2.203348053169E+00 2.261307556157E+00
H 1.953372520422E+01 -2.731735407685E+00 1.582995947354E+00
H 1.466057220422E+01 -3.057522443871E+00 7.872807708594E-01
H 9.787419204223E+00 -3.156547027629E+00 -6.682341883939E-02
H 4.914266204223E+00 -3.021464958590E+00 -9.159716212597E-01
H 4.111320422341E-02 -2.662294655854E+00 -1.697186398823E+00
H -4.832039795777E+00 -2.105674137682E+00 -2.352528625296E+00
H -9.705192795777E+00 -1.392885401536E+00 -2.833394565733E+00
H -1.457834579578E+01 -5.767927271843E-01 -3.104120593148E+00
H -1.945149879578E+01 2.820780250911E-01 -3.144628196576E+00
H -2.432465179578E+01 1.120028340667E+00 -2.951913112380E+00
H 2.684345470422E+01 1.874911278004E+00 -2.540268136743E+00
H 2.197030170422E+01 2.490740622999E+00 -1.940223094358E+00
H 1.709714870422E+01 2.921843130368E+00 -1.196280580994E+00
H 1.222399570422E+01 3.136245899299E+00 -3.636154095567E-01
H 7.350842704223E+00 3.118047657250E+00 4.960174533772E-01
H 2.477689704223E+00 2.868598084582E+00 1.318862970923E+00

PbE0/POB-TZVP optimized geometry, *all*-[-161.9]-$(PbMe_2)_\infty$

Energy (a.u): -6.5425565601968E+03
Unit cell length (Å): 58.03679770

Pb	-1.375211206315E+00	7.887551340354E-01	-2.709259628895E-01
Pb	-2.797541015215E+01	8.319997535914E-01	-5.754953395645E-02
Pb	3.461188602018E+00	8.185449648848E-01	1.597488006106E-01
Pb	-2.313901034382E+01	7.493076895308E-01	3.661605184135E-01
Pb	8.297588410351E+00	6.290063334248E-01	5.476190019953E-01
Pb	-1.830261053548E+01	4.658392351780E-01	6.917581555743E-01
Pb	1.313398821868E+01	2.709259628895E-01	7.887551340354E-01
Pb	-1.346621072715E+01	5.754953395645E-02	8.319997535914E-01
Pb	1.797038802702E+01	-1.597488006106E-01	8.185449648848E-01
Pb	-8.629810918815E+00	-3.661605184135E-01	7.493076895308E-01
Pb	2.280678783535E+01	-5.476190019953E-01	6.290063334248E-01
Pb	-3.793411110482E+00	-6.917581555743E-01	4.658392351780E-01
Pb	2.764318764368E+01	-7.887551340354E-01	2.709259628895E-01
Pb	1.042988697851E+00	-8.319997535914E-01	5.754953395645E-02
Pb	-2.555721024798E+01	-8.185449648848E-01	-1.597488006106E-01
Pb	5.879388506185E+00	-7.493076895308E-01	-3.661605184135E-01
Pb	-2.072081043965E+01	-6.290063334248E-01	-5.476190019953E-01
Pb	1.071578831452E+01	-4.658392351780E-01	-6.917581555743E-01
Pb	-1.588441063132E+01	-2.709259628895E-01	-7.887551340354E-01
Pb	1.555218812285E+01	-5.754953395645E-02	-8.319997535914E-01
Pb	-1.104801082298E+01	1.597488006106E-01	-8.185449648848E-01
Pb	2.038858793118E+01	3.661605184135E-01	-7.493076895308E-01
Pb	-6.211611014649E+00	5.476190019953E-01	-6.290063334248E-01
Pb	2.522498773952E+01	6.917581555743E-01	-4.658392351780E-01
C	-1.788828489874E+00	1.535773270803E+00	-2.352172544907E+00
C	-2.838902743571E+01	2.092230117582E+00	-1.874536837571E+00
C	3.047571318459E+00	2.506104939422E+00	-1.269154542572E+00
C	-2.355262762737E+01	2.749192851174E+00	-5.772814628747E-01
C	7.883971126792E+00	2.804927813375E+00	1.539323945150E-01
C	-1.871622781904E+01	2.669511580457E+00	8.746560136039E-01
C	1.272037093513E+01	2.352172544907E+00	1.535773270803E+00
C	-1.387982801071E+01	1.874536837571E+00	2.092230117582E+00
C	1.755677074346E+01	1.269154542572E+00	2.506104939422E+00
C	-9.043428202374E+00	5.772814628747E-01	2.749192851174E+00
C	2.239317055179E+01	-1.539323945150E-01	2.804927813375E+00
C	-4.207028394041E+00	-8.746560136039E-01	2.669511580457E+00
C	2.722957036013E+01	-1.535773270803E+00	2.352172544907E+00
C	6.293714142922E-01	-2.092230117582E+00	1.874536837571E+00
C	-2.597082753154E+01	-2.506104939422E+00	1.269154542572E+00
C	5.465771222626E+00	-2.749192851174E+00	5.772814628747E-01

C -2.113442772321E+01 -2.804927813375E+00 -1.539323945150E-01
C 1.030217103096E+01 -2.669511580457E+00 -8.746560136039E-01
C -1.629802791487E+01 -2.352172544907E+00 -1.535773270803E+00
C 1.513857083929E+01 -1.874536837571E+00 -2.092230117582E+00
C -1.146162810654E+01 -1.269154542572E+00 -2.506104939422E+00
C 1.997497064763E+01 -5.772814628747E-01 -2.749192851174E+00
C -6.625228298208E+00 1.539323945150E-01 -2.804927813375E+00
C 2.481137045596E+01 8.746560136039E-01 -2.669511580457E+00
C -1.421302657016E+00 2.662573170759E+00 9.730178908090E-01
C -2.802150160285E+01 2.320012628654E+00 1.628987755745E+00
C 3.415097151317E+00 1.819347059908E+00 2.173944797157E+00
C -2.318510179452E+01 1.194695995642E+00 2.570751093256E+00
C 8.251496959650E+00 4.886283736022E-01 2.792364950717E+00
C -1.834870198618E+01 -2.507384646023E-01 2.823683751387E+00
C 1.308789676798E+01 -9.730178908090E-01 2.662573170759E+00
C -1.351230217785E+01 -1.628987755745E+00 2.320012628654E+00
C 1.792429657632E+01 -2.173944797157E+00 1.819347059908E+00
C -8.675902369517E+00 -2.570751093256E+00 1.194695995642E+00
C 2.276069638465E+01 -2.792364950717E+00 4.886283736022E-01
C -3.839502561183E+00 -2.823683751387E+00 -2.507384646023E-01
C 2.759709619298E+01 -2.662573170759E+00 -9.730178908090E-01
C 9.968972471502E-01 -2.320012628654E+00 -1.628987755745E+00
C -2.560330169868E+01 -1.819347059908E+00 -2.173944797157E+00
C 5.833297055484E+00 -1.194695995642E+00 -2.570751093256E+00
C -2.076690189035E+01 -4.886283736022E-01 -2.792364950717E+00
C 1.066969686382E+01 2.507384646023E-01 -2.823683751387E+00
C -1.593050208202E+01 9.730178908090E-01 -2.662573170759E+00
C 1.550609667215E+01 1.628987755745E+00 -2.320012628654E+00
C -1.109410227368E+01 2.173944797157E+00 -1.819347059908E+00
C 2.034249648048E+01 2.570751093256E+00 -1.194695995642E+00
C -6.257702465350E+00 2.792364950717E+00 -4.886283736022E-01
C 2.517889628882E+01 2.823683751387E+00 2.507384646023E-01
H -1.965632056616E+00 7.071362539680E-01 -3.034171846413E+00
H -2.856583100245E+01 1.468342630379E+00 -2.747764617840E+00
H 2.870767751717E+00 2.129483883080E+00 -2.274101771457E+00
H -2.372943119412E+01 2.645504328288E+00 -1.645462647480E+00
H 7.707167560050E+00 2.981238025425E+00 -9.046879633332E-01
H -1.889303138578E+01 3.113805277859E+00 -1.022602895526E-01
H 1.254356736838E+01 3.034171846413E+00 7.071362539680E-01
H -1.405663157745E+01 2.747764617840E+00 1.468342630379E+00
H 1.737996717672E+01 2.274101771457E+00 2.129483883080E+00
H -9.220231769116E+00 1.645462647480E+00 2.645504328288E+00
H 2.221636698505E+01 9.046879633332E-01 2.981238025425E+00
H -4.383831960783E+00 1.022602895526E-01 3.113805277859E+00
H 2.705276679338E+01 -7.071362539680E-01 3.034171846413E+00

H 4.525678475502E-01 -1.468342630379E+00 2.747764617840E+00
H -2.614763109828E+01 -2.129483883080E+00 2.274101771457E+00
H 5.288967655884E+00 -2.645504328288E+00 1.645462647480E+00
H -2.131123128995E+01 -2.981238025425E+00 9.046879633332E-01
H 1.012536746422E+01 -3.113805277859E+00 1.022602895526E-01
H -1.647483148162E+01 -3.034171846413E+00 -7.071362539680E-01
H 1.496176727255E+01 -2.747764617840E+00 -1.468342630379E+00
H -1.163843167328E+01 -2.274101771457E+00 -2.129483883080E+00
H 1.979816708088E+01 -1.645462647480E+00 -2.645504328288E+00
H -6.802031864950E+00 -9.046879633332E-01 -2.981238025425E+00
H 2.463456688922E+01 -1.022602895526E-01 -3.113805277859E+00
H -9.396192622233E-01 2.113602854791E+00 -2.713614372798E+00
H -2.753981820806E+01 2.743918664705E+00 -2.074109532672E+00
H 3.896780546110E+00 3.187240952159E+00 -1.293257555522E+00
H -2.270341839972E+01 3.413358035889E+00 -4.242722131728E-01
H 8.733180354443E+00 3.406860410313E+00 4.736265793613E-01
H -1.786701859139E+01 3.168190877878E+00 1.339248503217E+00
H 1.356958016278E+01 2.713614372798E+00 2.113602854791E+00
H -1.303061878306E+01 2.074109532672E+00 2.743918664705E+00
H 1.840597997111E+01 1.293257555522E+00 3.187240952159E+00
H -8.194218974723E+00 4.242722131728E-01 3.413358035889E+00
H 2.324237977944E+01 -4.736265793613E-01 3.406860410313E+00
H -3.357819166390E+00 -1.339248503217E+00 3.168190877878E+00
H 2.807877958778E+01 -2.113602854791E+00 2.713614372798E+00
H 1.478580641943E+00 -2.743918664705E+00 2.074109532672E+00
H -2.512161830389E+01 -3.187240952159E+00 1.293257555522E+00
H 6.314980450277E+00 -3.413358035889E+00 4.242722131728E-01
H -2.028521849556E+01 -3.406860410313E+00 -4.736265793613E-01
H 1.115138025861E+01 -3.168190877878E+00 -1.339248503217E+00
H -1.544881868722E+01 -2.713614372798E+00 -2.113602854791E+00
H 1.598778006694E+01 -2.074109532672E+00 -2.743918664705E+00
H -1.061241887889E+01 -1.293257555522E+00 -3.187240952159E+00
H 2.082417987528E+01 -4.242722131728E-01 -3.413358035889E+00
H -5.776019070556E+00 4.736265793613E-01 -3.406860410313E+00
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H 2.167567974039E+00 3.052767957235E+00 -9.339685384796E-01
H -2.443263097179E+01 3.190476256846E+00 -1.120298446478E-01
H 7.003967782373E+00 3.110758872064E+00 7.175434979587E-01
H -1.959623116346E+01 2.819048410924E+00 1.498217436976E+00
H 1.184036759071E+01 2.335224459276E+00 2.176790333585E+00
H -1.475983135513E+01 1.692258819870E+00 2.707018566276E+00
H 1.667676739904E+01 9.339685384796E-01 3.052767957235E+00
H -9.923431546794E+00 1.120298446478E-01 3.190476256846E+00
H 2.151316720737E+01 -7.175434979587E-01 3.110758872064E+00
H -5.087031738461E+00 -1.498217436976E+00 2.819048410924E+00

H 2.634956701571E+01 -2.176790333585E+00 2.335224459276E+00
H -2.506319301273E-01 -2.707018566276E+00 1.692258819870E+00
H -2.685083087596E+01 -3.052767957235E+00 9.339685384796E-01
H 4.585767878206E+00 -3.190476256846E+00 1.120298446478E-01
H -2.201443106763E+01 -3.110758872064E+00 -7.175434979587E-01
H 9.422167686539E+00 -2.819048410924E+00 -1.498217436976E+00
H -1.717803125929E+01 -2.335224459276E+00 -2.176790333585E+00
H 1.425856749487E+01 -1.692258819870E+00 -2.707018566276E+00
H -1.234163145096E+01 -9.339685384796E-01 -3.052767957235E+00
H 1.909496730321E+01 -1.120298446478E-01 -3.190476256846E+00
H -7.505231642627E+00 7.175434979587E-01 -3.110758872064E+00
H 2.393136711154E+01 1.498217436976E+00 -2.819048410924E+00
H -2.668831834294E+00 2.176790333585E+00 -2.335224459276E+00
H 2.876776691987E+01 2.707018566276E+00 -1.692258819870E+00
H -6.044235730299E-01 3.317474372352E+00 6.731734527052E-01
H -2.720462251886E+01 3.030204064089E+00 1.508861172744E+00
H 4.231976235303E+00 2.536430356508E+00 2.241722497372E+00
H -2.236822271053E+01 1.869803111780E+00 2.821814138425E+00
H 9.068376043637E+00 1.075751874980E+00 3.209603809213E+00
H -1.753182290220E+01 2.083899256641E-01 3.378664284524E+00
H 1.390477585197E+01 -6.731734527052E-01 3.317474372352E+00
H -1.269542309386E+01 -1.508861172744E+00 3.030204064089E+00
H 1.874117566030E+01 -2.241722497372E+00 2.536430356508E+00
H -7.859023285530E+00 -2.821814138425E+00 1.869803111780E+00
H 2.357757546864E+01 -3.209603809213E+00 1.075751874980E+00
H -3.022623477197E+00 -3.378664284524E+00 2.083899256641E-01
H 2.841397527697E+01 -3.317474372352E+00 -6.731734527052E-01
H 1.813776331137E+00 -3.030204064089E+00 -1.508861172744E+00
H -2.478642261470E+01 -2.536430356508E+00 -2.241722497372E+00
H 6.650176139470E+00 -1.869803111780E+00 -2.821814138425E+00
H -1.995002280636E+01 -1.075751874980E+00 -3.209603809213E+00
H 1.148657594780E+01 -2.083899256641E-01 -3.378664284524E+00
H -1.511362299803E+01 6.731734527052E-01 -3.317474372352E+00
H 1.632297575614E+01 1.508861172744E+00 -3.030204064089E+00
H -1.027722318970E+01 2.241722497372E+00 -2.536430356508E+00
H 2.115937556447E+01 2.821814138425E+00 -1.869803111780E+00
H -5.440823381363E+00 3.209603809213E+00 -1.075751874980E+00
H 2.599577537280E+01 3.378664284524E+00 -2.083899256641E-01
H -1.314940846197E+00 2.429431301757E+00 2.030006093046E+00
H -2.791513979203E+01 1.821246199008E+00 2.589618402460E+00
H 3.521458962136E+00 1.088946177548E+00 2.972752497294E+00
H -2.307873998370E+01 2.824362736564E-01 3.153298422142E+00
H 8.357858770469E+00 -5.433211955365E-01 3.118952270594E+00
H -1.824234017536E+01 -1.332052223134E+00 2.872054676117E+00
H 1.319425857880E+01 -2.030006093046E+00 2.429431301757E+00

H -1.340594036703E+01 -2.589618402460E+00 1.821246199008E+00
H 1.803065838714E+01 -2.972752497294E+00 1.088946177548E+00
H -8.569540558697E+00 -3.153298422142E+00 2.824362736564E-01
H 2.286705819547E+01 -3.118952270594E+00 -5.433211955365E-01
H -3.733140750364E+00 -2.872054676117E+00 -1.332052223134E+00
H 2.770345800380E+01 -2.429431301757E+00 -2.030006093046E+00
H 1.103259057969E+00 -1.821246199008E+00 -2.589618402460E+00
H -2.549693988786E+01 -1.088946177548E+00 -2.972752497294E+00
H 5.939658866303E+00 -2.824362736564E-01 -3.153298422142E+00
H -2.066054007953E+01 5.433211955365E-01 -3.118952270594E+00
H 1.077605867464E+01 1.332052223134E+00 -2.872054676117E+00
H -1.582414027120E+01 2.030006093046E+00 -2.429431301757E+00
H 1.561245848297E+01 2.589618402460E+00 -1.821246199008E+00
H -1.098774046286E+01 2.972752497294E+00 -1.088946177548E+00
H 2.044885829130E+01 3.153298422142E+00 -2.824362736564E-01
H -6.151340654531E+00 3.118952270594E+00 5.433211955365E-01
H 2.528525809964E+01 2.872054676117E+00 1.332052223134E+00
H 2.471800168370E+00 2.347844320777E+00 2.300459785721E+00
H -2.412839877746E+01 1.672440660508E+00 2.829740344520E+00
H 7.308199976704E+00 8.830629330634E-01 3.166178775207E+00
H -1.929199896913E+01 3.350592606147E-02 3.286847354722E+00
H 1.214459978504E+01 -8.183344544304E-01 3.183522718784E+00
H -1.445559916080E+01 -1.614406694214E+00 2.863246270582E+00
H 1.698099959337E+01 -2.300459785721E+00 2.347844320777E+00
H -9.619199352463E+00 -2.829740344520E+00 1.672440660508E+00
H 2.181739940170E+01 -3.166178775207E+00 8.830629330634E-01
H -4.782799544130E+00 -3.286847354722E+00 3.350592606147E-02
H 2.665379921004E+01 -3.183522718784E+00 -8.183344544304E-01
H 5.360026420382E-02 -2.863246270582E+00 -1.614406694214E+00
H -2.654659868163E+01 -2.347844320777E+00 -2.300459785721E+00
H 4.890000072537E+00 -1.672440660508E+00 -2.829740344520E+00
H -2.171019887330E+01 -8.830629330634E-01 -3.166178775207E+00
H 9.726399880870E+00 -3.350592606147E-02 -3.286847354722E+00
H -1.687379906496E+01 8.183344544304E-01 -3.183522718784E+00
H 1.456279968920E+01 1.614406694214E+00 -2.863246270582E+00
H -1.203739925663E+01 2.300459785721E+00 -2.347844320777E+00
H 1.939919949754E+01 2.829740344520E+00 -1.672440660508E+00
H -7.200999448296E+00 3.166178775207E+00 -8.830629330634E-01
H 2.423559930587E+01 3.286847354722E+00 -3.350592606147E-02
H -2.364599639963E+00 3.183522718784E+00 8.183344544304E-01
H -2.896479858580E+01 2.863246270582E+00 1.614406694214E+00

PbE0/POB-TZVP optimized geometry, *all*-[148.7]-$(PbMe_2)_\infty$

Energy (a.u): -1.9082465331636E+03
Unit cell length (Å): 16.73777166

Pb -2.581379311088E+00 8.243057042269E-01 -2.971702490853E-01
Pb -7.363599785374E+00 7.462832565872E-01 4.591855310221E-01
Pb 4.591951400340E+00 1.062942953332E-01 8.697652405920E-01
Pb -1.902690739452E-01 -6.137364383152E-01 6.253939840186E-01
Pb -4.972489548231E+00 -8.716111159704E-01 -8.991169823324E-02
Pb 6.983061637483E+00 -4.731448456734E-01 -7.375120378510E-01
Pb 2.200841163198E+00 2.816091438117E-01 -8.297507704631E-01
C -1.963974051350E+00 1.537414961156E+00 -2.340409101376E+00
C -6.746194525636E+00 2.788368066816E+00 -2.572217886362E-01
C 5.209356660078E+00 1.939623145821E+00 2.019658777315E+00
C 4.271361857924E-01 -3.696975650792E-01 2.775695090417E+00
C -4.355084288493E+00 -2.400628469019E+00 1.441576386574E+00
C 7.600466897221E+00 -2.623837171891E+00 -9.780787391589E-01
C 2.818246422935E+00 -8.712429678047E-01 -2.661220625134E+00
C -2.583540344775E+00 2.715403276736E+00 9.222585309569E-01
C -7.365760819061E+00 9.719754965019E-01 2.698006558078E+00
C 4.589790366653E+00 -1.503369657285E+00 2.442100617662E+00
C -1.924301076325E-01 -2.846646795984E+00 3.472431023727E-01
C -4.974650581918E+00 -2.046340836295E+00 -2.009095551472E+00
C 6.980900603796E+00 2.949015108704E-01 -2.852544276978E+00
C 2.198680129510E+00 2.414077005456E+00 -1.547968980620E+00
H -1.694196395297E+00 6.985927674965E-01 -2.978501747917E+00
H -6.476416869583E+00 2.764251903294E+00 -1.310883645591E+00
H 5.479134316132E+00 2.748372975448E+00 1.343856579018E+00
H 6.969138418460E-01 6.629131404983E-01 2.986645389948E+00
H -4.085306632440E+00 -1.921733810211E+00 2.380429305784E+00
H 7.870244553275E+00 -3.059276005605E+00 -1.829859754368E-02
H 3.088024078989E+00 -1.893120970921E+00 -2.403247283698E+00
H -1.107531721281E+00 2.202123013018E+00 -2.240750434614E+00
H -5.889752195566E+00 3.124890475190E+00 3.246040553525E-01
H 6.065798990148E+00 1.694551673395E+00 2.645525070923E+00
H 1.283578515862E+00 -1.011819101021E+00 2.974311749211E+00
H -3.498641958424E+00 -2.956269455020E+00 1.063381015441E+00
H -8.280862432709E+00 -2.674588612482E+00 -1.648297311976E+00
H 3.674688753005E+00 -3.788879930800E-01 -3.118774144337E+00
H -2.781549899203E+00 2.084086434015E+00 -2.808054309836E+00
H -7.563770373489E+00 3.494831901710E+00 -1.213888389508E-01
H 4.391780812225E+00 2.273897665839E+00 2.656684903545E+00
H -3.904396620605E-01 -6.593278914685E-01 3.434220727176E+00
H -5.172660136346E+00 -3.096066098662E+00 1.625718297907E+00

H 6.782891049368E+00 -3.201403385324E+00 -1.406983168296E+00
H 2.000670575082E+00 -8.960186261093E-01 -3.380197611546E+00
H -3.320703988537E+00 3.405792502886E+00 5.145851762794E-01
H -8.102924462823E+00 1.721158001570E+00 2.983594411108E+00
H 3.852626722891E+00 -1.259543580153E+00 3.205896200137E+00
H -9.295937513946E-01 -3.291783156014E+00 1.014092762099E+00
H -5.711814225680E+00 -2.845242875257E+00 -1.941343209523E+00
H 6.243736960034E+00 -2.561766770538E-01 -3.434908148189E+00
H 1.461516485748E+00 2.525795784023E+00 -2.341917191912E+00
H -1.602596587055E+00 3.185200787468E+00 8.784721089947E-01
H -6.384817061341E+00 1.299123056577E+00 3.038008654800E+00
H 5.570734124374E+00 -1.565220833198E+00 2.909862719458E+00
H 7.885136500879E-01 -3.250921510888E+00 5.905308059820E-01
H -3.993706824198E+00 -2.488611984166E+00 -2.173482849032E+00
H 7.961844361516E+00 1.476731250664E-01 -3.300819587754E+00
H 3.179623887231E+00 2.672757359141E+00 -1.942571852449E+00
H -2.830672260897E+00 2.508813192087E+00 1.961206695990E+00
H -7.612892735183E+00 3.088630148281E-02 3.184261511492E+00
H 4.342658450531E+00 -2.470298604104E+00 2.009502461743E+00
H -4.395620237544E-01 -3.111298275892E+00 -6.784529280786E-01
H -5.221782498040E+00 -1.409426887015E+00 -2.855519425139E+00
H 6.733768687674E+00 1.353771694853E+00 -2.882321553089E+00
H 1.951548213388E+00 3.097552578587E+00 -7.386767629179E-01

PbE0/POB-TZVP optimized geometry, *all*-[-140.1]-$(PbMe_2)_\infty$

Energy (a.u): -5.9973508117098E+03
Unit cell length (Å): 52.34922886

Pb	-2.475620391567E+00	8.567428690801E-01	-2.689232423481E-01
Pb	-1.437317240520E+01	8.978031957375E-01	-1.665760241303E-02
Pb	2.607850444116E+01	8.661288469174E-01	2.369575374030E-01
Pb	1.418095242752E+01	7.642858899867E-01	4.713757867793E-01
Pb	2.283400413887E+00	6.005250356325E-01	6.676059732905E-01
Pb	-9.614151599749E+00	3.881132143512E-01	8.097506942514E-01
Pb	-2.151170361339E+01	1.442587686414E-01	8.862942297368E-01
Pb	1.893997323298E+01	-1.112826645639E-01	8.910354777236E-01
Pb	7.042421219342E+00	-3.578086381096E-01	8.235903304974E-01
Pb	-4.855130794295E+00	-5.753470837657E-01	6.894227927745E-01
Pb	-1.675268280793E+01	-7.462743304159E-01	4.994023205362E-01
Pb	2.369899403843E+01	-8.567428690801E-01	2.689232423481E-01
Pb	1.180144202480E+01	-8.978031957375E-01	1.665760241303E-02
Pb	-9.610998884002E-02	-8.661288469174E-01	-2.369575374030E-01
Pb	-1.199366200248E+01	-7.642858899867E-01	-4.713757867793E-01
Pb	-2.389121401611E+01	-6.005250356325E-01	-6.676059732905E-01
Pb	1.656046283025E+01	-3.881132143512E-01	-8.097506942514E-01
Pb	4.662910816614E+00	-1.442587686414E-01	-8.862942297368E-01
Pb	-7.234641197022E+00	1.112826645639E-01	-8.910354777236E-01
Pb	-1.913219321066E+01	3.578086381096E-01	-8.235903304974E-01
Pb	2.131948363571E+01	5.753470837657E-01	-6.894227927745E-01
Pb	9.421931622069E+00	7.462743304159E-01	-4.994023205362E-01
C	-2.587023626905E+00	1.629016735517E+00	-2.379357946497E+00
C	-1.448457564054E+01	2.233372709537E+00	-1.824030181343E+00
C	2.596710120582E+01	2.656794109008E+00	-1.120930338822E+00
C	1.406954919219E+01	2.864977850331E+00	-3.270193866786E-01
C	2.171997178549E+00	2.841058124900E+00	4.933847313140E-01
C	-9.725554835087E+00	2.586972766612E+00	1.273817752648E+00
C	-2.162310684872E+01	2.123306260093E+00	1.951053635348E+00
C	1.882856999764E+01	1.487622108170E+00	2.470226755874E+00
C	6.931017984004E+00	7.314196602717E-01	2.789276795645E+00
C	-4.966534029633E+00	-8.403805858118E-02	2.882356217899E+00
C	-1.686408604327E+01	-8.926875137214E-01	2.741924281412E+00
C	2.358759080309E+01	-1.629016735517E+00	2.379357946497E+00
C	1.169003878946E+01	-2.233372709537E+00	1.824030181343E+00
C	-2.075132241780E-01	-2.656794109008E+00	1.120930338822E+00
C	-1.210506523781E+01	-2.864977850331E+00	3.270193866786E-01
C	-2.400261725145E+01	-2.841058124900E+00	-4.933847313140E-01
C	1.644905959491E+01	-2.586972766612E+00	-1.273817752648E+00
C	4.551507581276E+00	-2.123306260093E+00	-1.951053635348E+00

C -7.346044432360E+00 -1.487622108170E+00 -2.470226755874E+00
C -1.924359644600E+01 -7.314196602717E-01 -2.789276795645E+00
C 2.120808040037E+01 8.403805858118E-02 -2.882356217899E+00
C 9.310528386731E+00 8.926875137214E-01 -2.741924281412E+00
C -1.833530894026E+00 2.664650499966E+00 9.077009881425E-01
C -1.373108290766E+01 2.300984511619E+00 1.621651518710E+00
C -2.562863492130E+01 1.750906442622E+00 2.204225487564E+00
C 1.482304192506E+01 1.058980346686E+00 2.608226216450E+00
C 2.925489911428E+00 2.812619610595E-01 2.800923968998E+00
C -8.972062102208E+00 -5.192425959225E-01 2.766707519313E+00
C -2.086961411584E+01 -1.277681205837E+00 2.508348880657E+00
C 1.958206273052E+01 -1.932609683118E+00 2.046778733415E+00
C 7.684510716883E+00 -2.430969617545E+00 1.419390745854E+00
C -4.213041296753E+00 -2.732386851091E+00 6.770121615059E-01
C -1.611059331039E+01 -2.812442352093E+00 -1.202139218214E-01
C 2.434108353597E+01 -2.664650499966E+00 -9.077009881425E-01
C 1.244353152234E+01 -2.300984511619E+00 -1.621651518710E+00
C 5.459795087011E-01 -1.750906442622E+00 -2.204225487564E+00
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C -2.324912451857E+01 -2.812619610595E-01 -2.800923968998E+00
C 1.720255232779E+01 5.192425959225E-01 -2.766707519313E+00
C 5.305000314156E+00 1.277681205837E+00 -2.508348880657E+00
C -6.592551699481E+00 1.932609683118E+00 -2.046778733415E+00
C -1.849010371312E+01 2.430969617545E+00 -1.419390745854E+00
C 2.196157313325E+01 2.732386851091E+00 -6.770121615059E-01
C 1.006402111961E+01 2.812442352093E+00 1.202139218214E-01
H -2.854200563093E+00 8.316923318929E-01 -3.069706647858E+00
H -1.475175257673E+01 1.662839251314E+00 -2.711047152508E+00
H 2.569992426963E+01 2.359272823880E+00 -2.132754740080E+00
H 1.380237225600E+01 2.864572143391E+00 -1.381679222591E+00
H 1.904820242362E+00 3.137800864111E+00 -5.186682716511E-01
H -9.992731771275E+00 3.156823620041E+00 3.863620980192E-01
H -2.189028378491E+01 2.920099300628E+00 1.260091708292E+00
H 1.856139306145E+01 2.446805902377E+00 2.031736182413E+00
H 6.663841047816E+00 1.775286841631E+00 2.638781474235E+00
H -5.233710965820E+00 9.599445990133E-01 3.032048384452E+00
H -1.713126297946E+01 6.683335399387E-02 3.179676766847E+00
H 2.332041386691E+01 -8.316923318929E-01 3.069706647858E+00
H 1.142286185327E+01 -1.662839251314E+00 2.711047152508E+00
H -4.746901603656E-01 -2.359272823880E+00 2.132754740080E+00
H -1.237224217400E+01 -2.864572143391E+00 1.381679222591E+00
H -2.426979418764E+01 -3.137800864111E+00 5.186682716511E-01
H 1.618188265873E+01 -3.156823620041E+00 -3.863620980192E-01
H 4.284330645089E+00 -2.920099300628E+00 -1.260091708292E+00
H -7.613221368547E+00 -2.446805902377E+00 -2.031736182413E+00

H -1.951077338218E+01 -1.775286841631E+00 -2.638781474235E+00
H 2.094090346418E+01 -9.599445990133E-01 -3.032048384452E+00
H 9.043351450543E+00 -6.683335399387E-02 -3.179676766847E+00
H -1.625055840732E+00 2.043976714605E+00 -2.675117018067E+00
H -1.352260785437E+01 2.714848853245E+00 -1.990901196502E+00
H -2.542015986800E+01 3.165780083623E+00 -1.145394400341E+00
H 1.503151697836E+01 3.360238639245E+00 -2.070945617881E-01
H 3.133964964723E+00 3.282470644424E+00 7.479828465224E-01
H -8.763587048914E+00 2.938776399597E+00 1.642463133033E+00
H -2.066113906255E+01 2.356999968450E+00 2.403880824610E+00
H 1.979053778381E+01 1.584273417478E+00 2.970550388206E+00
H 7.892985770177E+00 6.831984562587E-01 3.296563625894E+00
H -4.004566243459E+00 -2.732251807490E-01 3.355508884030E+00
H -1.590211825710E+01 -1.207513738545E+00 3.142610768362E+00
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H 1.265200657563E+01 -2.714848853245E+00 1.990901196502E+00
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H -1.828162865982E+01 -6.831984562587E-01 -3.296563625894E+00
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H 2.521319133737E+01 3.346191385681E+00 -7.437482975255E-01
H 1.331563932373E+01 3.420185232439E+00 2.291097891552E-01
H 1.418087310096E+00 3.217096012289E+00 1.183406763287E+00
H -1.047946470354E+01 2.753376806030E+00 2.041831159448E+00
H -2.237701671718E+01 2.066595385909E+00 2.734838538308E+00
H 1.807466012919E+01 1.212390698138E+00 3.206285563506E+00
H 6.177108115551E+00 2.599653263686E-01 3.417978400863E+00
H -5.720443898086E+00 -7.135208900698E-01 3.352766955682E+00
H -1.761799591172E+01 -1.629201887467E+00 3.015934271424E+00
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H -1.455171765779E+01 2.965926010772E+00 1.887027596590E+00
H 2.589995918858E+01 2.314148057979E+00 2.646187638362E+00
H 1.400240717494E+01 1.474891592297E+00 3.190969295158E+00
H 2.104855161305E+00 5.161481813245E-01 3.477237597085E+00
H -9.792696852332E+00 -4.844104856471E-01 3.481800788825E+00
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H -1.693122806051E+01 -3.515299877060E+00 1.603203079590E-02
H 2.352044878585E+01 -3.377422277214E+00 -9.749918015269E-01
H 1.162289677221E+01 -2.965926010772E+00 -1.887027596590E+00
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H -7.413186449604E+00 2.289915657079E+00 -2.667185133269E+00
H -1.931073846324E+01 2.948590870302E+00 -1.914001601681E+00
H 2.114093838312E+01 3.368388787159E+00 -1.005757043330E+00
H 9.243386369486E+00 3.515299877060E+00 -1.603203079590E-02
H -9.943554212986E-01 3.138022831040E+00 4.011898045870E-01
H -1.289190743493E+01 2.897882628000E+00 1.269021994203E+00
H -2.478945944857E+01 2.422973208811E+00 2.034045569012E+00
H 1.566221739779E+01 1.751768910220E+00 2.634282868756E+00
H 3.764665384156E+00 9.386467126943E-01 3.021106237156E+00
H -8.132886629480E+00 4.948094085310E-02 3.163177545432E+00
H -2.003043864312E+01 -8.436934825416E-01 3.048987021119E+00
H 2.042123820325E+01 -1.668516877619E+00 2.687785701378E+00
H 8.523686189611E+00 -2.358166958324E+00 2.108835968989E+00
H -3.373865824026E+00 -2.856772376624E+00 1.359040888123E+00
H -1.527141783766E+01 -3.123939086850E+00 4.991443970287E-01
H 2.518025900870E+01 -3.138022831040E+00 -4.011898045870E-01
H 1.328270699507E+01 -2.897882628000E+00 -1.269021994203E+00
H 1.385154981429E+00 -2.422973208811E+00 -2.034045569012E+00
H -1.051239703221E+01 -1.751768910220E+00 -2.634282868756E+00
H -2.240994904584E+01 -9.386467126943E-01 -3.021106237156E+00
H 1.804172780052E+01 -4.948094085310E-02 -3.163177545432E+00
H 6.144175786883E+00 8.436934825416E-01 -3.048987021119E+00
H -5.753376226753E+00 1.668516877619E+00 -2.687785701378E+00
H -1.765092824039E+01 2.358166958324E+00 -2.108835968989E+00
H 2.280074860597E+01 2.856772376624E+00 -1.359040888123E+00

H 1.090319659234E+01 3.123939086850E+00 -4.991443970287E-01
H -1.531999395720E+00 2.382817451479E+00 1.914428784654E+00
H -1.342955140936E+01 1.746939685709E+00 2.508198220452E+00
H -2.532710342299E+01 9.695352560526E-01 2.898768353259E+00
H 1.512457342337E+01 1.135848459994E-01 3.054497513724E+00
H 3.227021409734E+00 -7.515675327617E-01 2.962769451423E+00
H -8.670530603902E+00 -1.555832379763E+00 2.631015428436E+00
H -2.056808261754E+01 -2.234052940247E+00 2.086112182688E+00
H 1.988359422883E+01 -2.731283817936E+00 1.372204534486E+00
H 7.986042215189E+00 -3.007242324267E+00 5.471290357147E-01
H -3.911509798448E+00 -3.039571942244E+00 -3.222716036288E-01
H -1.580906181208E+01 -2.825653518492E+00 -1.165563714269E+00
H 2.464261503428E+01 -2.382817451479E+00 -1.914428784654E+00
H 1.274506302064E+01 -1.746939685709E+00 -2.508198220452E+00
H 8.475110070068E-01 -9.695352560526E-01 -2.898768353259E+00
H -1.105004100663E+01 -1.135848459994E-01 -3.054497513724E+00
H -2.294759302027E+01 7.515675327617E-01 -2.962769451423E+00
H 1.750408382610E+01 1.555832379763E+00 -2.631015428436E+00
H 5.606531812461E+00 2.234052940247E+00 -2.086112182688E+00
H -6.291020201175E+00 2.731283817936E+00 -1.372204534486E+00
H -1.818857221481E+01 3.007242324267E+00 -5.471290357147E-01
H 2.226310463155E+01 3.039571942244E+00 3.222716036288E-01
H 2.226310463155E+01 3.039571942244E+00 3.222716036288E-01
H 1.036555261792E+01 2.825653518492E+00 1.165563714269E+00

PbE0/POB-TZVP optimized geometry, *all*-[-129.8]-$(PbMe_2)_\infty$

Energy (a.u): -3.5438889985921E+03
Unit cell length (Å): 30.85998318

Pb	-2.490274329851E+00	8.728974178465E-01	-2.918574038514E-01
Pb	9.378949970149E+00	9.085451769116E-01	1.472287600187E-01
Pb	-9.611808909851E+00	7.360561851026E-01	5.525865892674E-01
Pb	2.257415390149E+00	3.949455917252E-01	8.313534903053E-01
Pb	1.412663969015E+01	-3.664227710612E-02	9.196673256099E-01
Pb	-4.864119189851E+00	-4.598358418397E-01	7.972964598100E-01
Pb	7.005105110149E+00	-7.776865568304E-01	4.922745835316E-01
Pb	-1.198565376985E+01	-9.173786537903E-01	7.447853271790E-02
Pb	-1.164294698513E-01	-8.469103567781E-01	-3.603796523778E-01
Pb	1.175279483015E+01	-5.824251034042E-01	-7.126792021594E-01
Pb	-7.237964049851E+00	-1.845132778238E-01	-9.017125354417E-01
Pb	4.631260250149E+00	2.556683160799E-01	-8.841743936684E-01
Pb	-1.435949862985E+01	6.372793799070E-01	-6.640825537622E-01
C	-2.717380374631E+00	1.615333516253E+00	-2.403461057260E+00
C	9.151843925369E+00	2.547250841819E+00	-1.377476159992E+00
C	-9.838914954631E+00	2.895623697225E+00	-3.592807485711E-02
C	2.030309345369E+00	2.580644059645E+00	1.313850699247E+00
C	1.389953364537E+01	1.674469968133E+00	2.362642111772E+00
C	-5.091225234631E+00	3.846949864721E-01	2.870180689413E+00
C	6.777999065369E+00	-9.932089805124E-01	2.720195460537E+00
C	-1.221275981463E+01	-2.143580739527E+00	1.947046233561E+00
C	-3.435355146307E-01	-2.802883984065E+00	7.278521789266E-01
C	1.152568878537E+01	-2.820080286267E+00	-6.580840383299E-01
C	-7.465070094631E+00	-2.191230180537E+00	-1.893261133177E+00
C	4.404154205369E+00	-1.060395647632E+00	-2.694714918684E+00
C	-1.458660467463E+01	3.133627489923E-01	-2.878841991155E+00
C	-1.893923997460E+00	2.702226910958E+00	8.752205641060E-01
C	9.975300302540E+00	1.985967824201E+00	2.030756783906E+00
C	-9.015458577460E+00	8.147474424259E-01	2.721071097785E+00
C	2.853765722540E+00	-5.431217596377E-01	2.788020815623E+00
C	1.472299002254E+01	-1.776568311895E+00	2.216268563895E+00
C	-4.267768857460E+00	-2.603024473866E+00	1.136795893111E+00
C	7.601455442540E+00	-2.833159098720E+00	-2.031030169101E-01
C	-1.138930343746E+01	-2.414251117326E+00	-1.496473473413E+00
C	4.799208625399E-01	-1.442267299832E+00	-2.447019891618E+00
C	1.234914516254E+01	-1.398774251522E-01	-2.836983542439E+00
C	-6.641613717460E+00	1.194556681925E+00	-2.577028453046E+00
C	5.227610582540E+00	2.255332249141E+00	-1.726707201619E+00
C	-1.376314829746E+01	2.799438377779E+00	-4.808181393792E-01
H	-2.867221242599E+00	7.810224913167E-01	-3.085638135900E+00

H 9.002003057401E+00 2.125528613402E+00 -2.369237630816E+00
H -9.988755822599E+00 2.983101745553E+00 -1.110073336920E+00
H 1.880468477401E+00 3.157282218071E+00 4.033953806296E-01
H 1.374969277740E+01 2.608167383805E+00 1.824451077919E+00
H -5.241066102599E+00 1.461552833733E+00 2.827547020276E+00
H 6.628158197401E+00 -1.988585692573E-02 3.182886015923E+00
H -1.236260068260E+01 -1.496768937414E+00 2.809064183257E+00
H -4.933763825988E-01 -2.630760292361E+00 1.791719599100E+00
H 1.137584791740E+01 -3.162076168427E+00 3.639136473512E-01
H -7.614910962599E+00 -2.968998501455E+00 -1.147260535371E+00
H 4.254313337401E+00 -2.095759058111E+00 -2.395611155428E+00
H -1.473644554260E+01 -7.424064711876E-01 -3.095156130020E+00
H -1.822842201499E+00 2.158643529190E+00 -2.703361946872E+00
H 1.004638209850E+01 3.167698859291E+00 -1.390536457182E+00
H -8.944376781499E+00 3.451072555639E+00 2.408441770666E-01
H 2.924847518501E+00 2.943847119422E+00 1.817050312837E+00
H 1.479407181850E+01 1.762221785349E+00 2.976992119766E+00
H -4.196687061499E+00 1.768926773281E-01 3.454940908701E+00
H 7.672537238501E+00 -1.448960411281E+00 3.141404372004E+00
H -1.131822164150E+01 -2.742874131532E+00 2.108209951708E+00
H 5.510026585007E-01 -3.408428443465E+00 5.920500381597E-01
H 1.242022695850E+01 -3.293152875017E+00 -1.059741404155E+00
H -6.570531921499E+00 -2.423455669696E+00 -2.468758862046E+00
H 5.298692378501E+00 -9.985739762544E-01 -3.312213416412E+00
H -1.369206650150E+01 6.550689810258E-01 -3.396879793576E+00
H -3.575647490828E+00 2.282008502316E+00 -2.467678024687E+00
H 8.293576809172E+00 3.167405338183E+00 -1.124518146504E+00
H -1.069718207083E+01 3.327187782444E+00 4.762552871304E-01
H 1.172042229172E+00 2.724751602707E+00 1.967924373982E+00
H 1.304126652917E+01 1.498107667606E+00 3.008765702813E+00
H -5.949492350828E+00 -7.173467998852E-02 3.360335068688E+00
H 5.919731949172E+00 -1.625143476895E+00 2.942092166754E+00
H -1.307102693083E+01 -2.806251488346E+00 1.849851405470E+00
H -1.201802630828E+00 -3.344481102814E+00 3.338319803200E-01
H 1.066742166917E+01 -3.116530401994E+00 -1.258664328410E+00
H -8.323337210828E+00 -2.174620144340E+00 -2.562815808051E+00
H 3.545887089172E+00 -7.345306186312E-01 -3.279857071346E+00
H 1.541511138917E+01 8.738310197523E-01 -3.245522606158E+00
H -2.699438202767E+00 3.434797003804E+00 8.545461977559E-01
H 9.169786097233E+00 2.644234284235E+00 2.352892838936E+00
H -9.820972782767E+00 1.247909356625E+00 3.312220086149E+00
H 2.048251517233E+00 -4.342965656496E-01 3.512757628204E+00
H 1.391747581723E+01 -2.017010378575E+00 2.908564730956E+00
H -5.073283062767E+00 -3.137651421379E+00 1.638054705851E+00
H 6.795941237233E+00 -3.539494336343E+00 -7.713911665367E-03

H -1.219481764277E+01 -3.130481754383E+00 -1.651715364982E+00
H -3.255933427665E-01 -2.004313528888E+00 -2.917328733509E+00
H 1.154363095723E+01 -4.189812285211E-01 -3.514617246812E+00
H -7.447127922767E+00 1.262334622028E+00 -3.306749304599E+00
H 4.422096377233E+00 2.654464823453E+00 -2.341344947352E+00
H -1.456866250277E+01 3.438489123593E+00 -8.395666789322E-01
H -1.002789539258E+00 3.142530466877E+00 4.317198087832E-01
H 1.086643476074E+01 2.581942338723E+00 1.842675632892E+00
H -8.124324119258E+00 1.429862336546E+00 2.831496676154E+00
H 3.744900180742E+00 -4.978189522443E-02 3.171655954143E+00
H -1.524585869926E+01 -1.518021694736E+00 2.785227075636E+00
H -3.376634399258E+00 -2.638501018128E+00 1.760736239726E+00
H 8.492589900742E+00 -3.154531555651E+00 3.328819504658E-01
H -1.049816897926E+01 -2.947896930001E+00 -1.171231581983E+00
H 1.371055320742E+00 -2.065934643697E+00 -2.407030073871E+00
H 1.324027962074E+01 -7.106916277333E-01 -3.091406983691E+00
H -5.750479259258E+00 8.073622753816E-01 -3.067579809041E+00
H 6.118745040742E+00 2.140459210977E+00 -2.341007068484E+00
H -1.287201383926E+01 2.983202736667E+00 -1.078137820730E+00
H -1.684838855886E+00 2.441142045387E+00 1.910582569995E+00
H 1.018438544411E+01 1.273631941184E+00 2.826192123852E+00
H -8.806373435886E+00 -1.856518918160E-01 3.094355121441E+00
H 3.062850864114E+00 -1.602405113748E+00 2.653638651730E+00
H 1.493207516411E+01 -2.652066635196E+00 1.605005546721E+00
H -4.058683715886E+00 -3.094171651388E+00 1.886850133708E-01
H 7.810540584114E+00 -2.827439231058E+00 -1.270860982641E+00
H -1.118021829589E+01 -1.912974557229E+00 -2.439268043066E+00
H 6.890060041140E-01 -5.602704661809E-01 -3.048868191190E+00
H 1.255823030411E+01 9.207848366777E-01 -2.960009379558E+00
H -6.432528575886E+00 2.190899430114E+00 -2.193048091049E+00
H 5.436695724114E+00 2.959105367311E+00 -9.236859139750E-01
H -1.355406315589E+01 3.049415925943E+00 5.572815743684E-01

PbE0/POB-TZVP optimized geometry, *all*-[-113.9]-$(PbMe_2)_\infty$

Energy (a.u): -5.4521334021154E+03
Unit cell length (Å): 45.93386173

Pb	-2.519914634527E+00	9.708697224754E-01	-3.205122478045E-01
Pb	-9.409993894027E+00	1.022395707511E+00	-4.810018257889E-03
Pb	-1.630007315353E+01	9.738424772453E-01	3.113630493892E-01
Pb	2.274370931697E+01	8.299627601475E-01	5.970577323681E-01
Pb	1.585363005747E+01	6.048405053959E-01	8.243082445570E-01
Pb	8.963550797973E+00	3.205122478045E-01	9.708697224754E-01
Pb	2.073471538473E+00	4.810018257889E-03	1.022395707511E+00
Pb	-4.816607721027E+00	-3.113630493892E-01	9.738424772453E-01
Pb	-1.170668698053E+01	-5.970577323681E-01	8.299627601475E-01
Pb	-1.859676624003E+01	-8.243082445570E-01	6.048405053959E-01
Pb	2.044701623047E+01	-9.708697224754E-01	3.205122478045E-01
Pb	1.355693697097E+01	-1.022395707511E+00	4.810018257890E-03
Pb	6.666857711473E+00	-9.738424772453E-01	-3.113630493892E-01
Pb	-2.232215480274E-01	-8.299627601475E-01	-5.970577323681E-01
Pb	-7.113300807527E+00	-6.048405053959E-01	-8.243082445570E-01
Pb	-1.400338006703E+01	-3.205122478045E-01	-9.708697224754E-01
Pb	-2.089345932653E+01	-4.810018257890E-03	-1.022395707511E+00
Pb	1.815032314397E+01	3.113630493892E-01	-9.738424772453E-01
Pb	1.126024388447E+01	5.970577323681E-01	-8.299627601475E-01
Pb	4.370164624972E+00	8.243082445570E-01	-6.048405053959E-01
C	-2.915514175169E+00	1.742073365252E+00	-2.397032047810E+00
C	-9.805593434669E+00	2.397533864722E+00	-1.741382673527E+00
C	-1.669567269417E+01	2.818307044912E+00	-9.152746302330E-01
C	2.234810977633E+01	2.963204695246E+00	4.268709616790E-04
C	1.545803051683E+01	2.818043224149E+00	9.160865870525E-01
C	8.567951257331E+00	2.397032047810E+00	1.742073365252E+00
C	1.677871997831E+00	1.741382673527E+00	2.397533864722E+00
C	-5.212207261669E+00	9.152746302330E-01	2.818307044912E+00
C	-1.210228652117E+01	-4.268709616786E-04	2.963204695246E+00
C	-1.899236578067E+01	-9.160865870525E-01	2.818043224149E+00
C	2.005141668983E+01	-1.742073365252E+00	2.397032047810E+00
C	1.316133743033E+01	-2.397533864722E+00	1.741382673527E+00
C	6.271258170831E+00	-2.818307044912E+00	9.152746302330E-01
C	-6.188210886692E-01	-2.963204695246E+00	-4.268709616781E-04
C	-7.508900348169E+00	-2.818043224149E+00	-9.160865870525E-01
C	-1.439897960767E+01	-2.397032047810E+00	-1.742073365252E+00
C	-2.128905886717E+01	-1.741382673527E+00	-2.397533864722E+00
C	1.775472360333E+01	-9.152746302330E-01	-2.818307044912E+00
C	1.086464434383E+01	4.268709616779E-04	-2.963204695246E+00
C	3.974565084331E+00	9.160865870525E-01	-2.818043224149E+00

C	-1.733318203432E+00	2.771329158984E+00	7.779927786213E-01
C	-8.623397462932E+00	2.395277665356E+00	1.596302908871E+00
C	-1.551347672243E+01	1.784759704961E+00	2.258355788305E+00
C	-2.240355598193E+01	9.995370294933E-01	2.699345068289E+00
C	1.664022648857E+01	1.164727053945E-01	2.876103645545E+00
C	9.750147229068E+00	-7.779927786213E-01	2.771329158984E+00
C	2.860067969568E+00	-1.596302908871E+00	2.395277665356E+00
C	-4.030011289932E+00	-2.258355788305E+00	1.784759704961E+00
C	-1.092009054943E+01	-2.699345068289E+00	9.995370294933E-01
C	-1.781016980893E+01	-2.876103645545E+00	1.164727053945E-01
C	2.123361266157E+01	-2.771329158984E+00	-7.779927786213E-01
C	1.434353340207E+01	-2.395277665356E+00	-1.596302908871E+00
C	7.453454142568E+00	-1.784759704961E+00	-2.258355788305E+00
C	5.633748830678E-01	-9.995370294933E-01	-2.699345068289E+00
C	-6.326704376432E+00	-1.164727053945E-01	-2.876103645545E+00
C	-1.321678363593E+01	7.779927786213E-01	-2.771329158984E+00
C	-2.010686289543E+01	1.596302908871E+00	-2.395277665356E+00
C	1.893691957507E+01	2.258355788305E+00	-1.784759704961E+00
C	1.204684031557E+01	2.699345068289E+00	-9.995370294933E-01
C	5.156761056068E+00	2.876103645545E+00	-1.164727053945E-01
H	-3.262777190880E+00	9.400251778920E-01	-3.044238259365E+00
H	-1.015285645038E+01	1.834738427986E+00	-2.604758878615E+00
H	-1.704293570988E+01	2.549854697374E+00	-1.910307550404E+00
H	2.200084676062E+01	3.015373423101E+00	-1.028862009264E+00
H	1.511076750112E+01	3.185726388833E+00	-4.670428615450E-02
H	8.220688241620E+00	3.044238259365E+00	9.400251778920E-01
H	1.330608982120E+00	2.604758878615E+00	1.834738427986E+00
H	-5.559470277380E+00	1.910307550404E+00	2.549854697374E+00
H	-1.244954953688E+01	1.028862009264E+00	3.015373423101E+00
H	-1.933962879638E+01	4.670428615450E-02	3.185726388833E+00
H	1.970415367412E+01	-9.400251778920E-01	3.044238259365E+00
H	1.281407441462E+01	-1.834738427986E+00	2.604758878615E+00
H	5.923995155120E+00	-2.549854697374E+00	1.910307550404E+00
H	-9.660841043804E-01	-3.015373423101E+00	1.028862009264E+00
H	-7.856163363880E+00	-3.185726388833E+00	4.670428615450E-02
H	-1.474624262338E+01	-3.044238259365E+00	-9.400251778920E-01
H	-2.163632188288E+01	-2.604758878615E+00	-1.834738427986E+00
H	1.740746058762E+01	-1.910307550404E+00	-2.549854697374E+00
H	1.051738132812E+01	-1.028862009264E+00	-3.015373423101E+00
H	3.627302068619E+00	-4.670428615450E-02	-3.185726388833E+00
H	-2.004390193322E+00	2.166950096827E+00	-2.814653558140E+00
H	-8.894469452822E+00	2.930667792817E+00	-2.007270201700E+00
H	-1.578454871232E+01	3.407511306083E+00	-1.003401252445E+00
H	-2.267462797182E+01	3.550803871182E+00	9.868760250825E-02
H	1.636915449868E+01	3.346519013464E+00	1.191116227331E+00

H 9.479075239178E+00 2.814653558140E+00 2.166950096827E+00
H 2.588995979678E+00 2.007270201700E+00 2.930667792817E+00
H -4.301083279822E+00 1.003401252445E+00 3.407511306083E+00
H -1.119116253932E+01 -9.868760250825E-02 3.550803871182E+00
H -1.808124179882E+01 -1.191116227331E+00 3.346519013464E+00
H 2.096254067168E+01 -2.166950096827E+00 2.814653558140E+00
H 1.407246141218E+01 -2.930667792817E+00 2.007270201700E+00
H 7.182382152678E+00 -3.407511306083E+00 1.003401252445E+00
H 2.923028931780E-01 -3.550803871182E+00 -9.868760250825E-02
H -6.597776366322E+00 -3.346519013464E+00 -1.191116227331E+00
H -1.348785562582E+01 -2.814653558140E+00 -2.166950096827E+00
H -2.037793488532E+01 -2.007270201700E+00 -2.930667792817E+00
H 1.866584758518E+01 -1.003401252445E+00 -3.407511306083E+00
H 1.177576832568E+01 9.868760250825E-02 -3.550803871182E+00
H 4.885689066178E+00 1.191116227331E+00 -3.346519013464E+00
H -3.678495624310E+00 2.518343344624E+00 -2.355905323192E+00
H -1.056857488381E+01 3.123101630178E+00 -1.462388218236E+00
H -1.745865414331E+01 3.422148968241E+00 -4.257223654218E-01
H 2.158512832719E+01 3.386212521780E+00 6.526161587023E-01
H 1.469504906769E+01 3.018810000556E+00 1.667072066168E+00
H 7.804969808190E+00 2.355905323192E+00 2.518343344624E+00
H 9.148905486901E-01 1.462388218236E+00 3.123101630178E+00
H -5.975188710810E+00 4.257223654218E-01 3.422148968241E+00
H -1.286526797031E+01 -6.526161587023E-01 3.386212521780E+00
H -1.975534722981E+01 -1.667072066168E+00 3.018810000556E+00
H 1.928843524069E+01 -2.518343344624E+00 2.355905323192E+00
H 1.239835598119E+01 -3.123101630178E+00 1.462388218236E+00
H 5.508276721690E+00 -3.422148968241E+00 4.257223654218E-01
H -1.381802537810E+00 -3.386212521780E+00 -6.526161587023E-01
H -8.271881797310E+00 -3.018810000556E+00 -1.667072066168E+00
H -1.516196105681E+01 -2.355905323192E+00 -2.518343344624E+00
H -2.205204031631E+01 -1.462388218236E+00 -3.123101630178E+00
H 1.699174215419E+01 -4.257223654218E-01 -3.422148968241E+00
H 1.010166289469E+01 6.526161587023E-01 -3.386212521780E+00
H 3.211583635190E+00 1.667072066168E+00 -3.018810000556E+00
H -2.523318629512E+00 3.512222336277E+00 8.907863304836E-01
H -9.413397889012E+00 3.065053825117E+00 1.932524534166E+00
H -1.630347714851E+01 2.317856490069E+00 2.785093771754E+00
H 2.274030532199E+01 1.343771212318E+00 3.365038626073E+00
H 1.585022606249E+01 2.381482456998E-01 3.615590054070E+00
H 8.960146802988E+00 -8.907863304836E-01 3.512222336277E+00
H 2.070067543488E+00 -1.932524534166E+00 3.065053825117E+00
H -4.820011716012E+00 -2.785093771754E+00 2.317856490069E+00
H -1.171009097551E+01 -3.365038626073E+00 1.343771212318E+00
H -1.860017023501E+01 -3.615590054070E+00 2.381482456998E-01

H 2.044361223549E+01 -3.512222336277E+00 -8.907863304836E-01
H 1.355353297599E+01 -3.065053825117E+00 -1.932524534166E+00
H 6.663453716488E+00 -2.317856490069E+00 -2.785093771754E+00
H -2.266255430118E-01 -1.343771212318E+00 -3.365038626073E+00
H -7.116704802512E+00 -2.381482456998E-01 -3.615590054070E+00
H -1.400678406201E+01 8.907863304836E-01 -3.512222336277E+00
H -2.089686332151E+01 1.932524534166E+00 -3.065053825117E+00
H 1.814691914899E+01 2.785093771754E+00 -2.317856490069E+00
H 1.125683988949E+01 3.365038626073E+00 -1.343771212318E+00
H 4.366760629988E+00 3.615590054070E+00 -2.381482456998E-01
H -9.159167202474E-01 3.211520795099E+00 2.089190202808E-01
H -7.805995979747E+00 2.989778251681E+00 1.191108299090E+00
H -1.469607523925E+01 2.475375381979E+00 2.056703598645E+00
H -2.158615449875E+01 1.718665522934E+00 2.720974420068E+00
H 1.745762797175E+01 7.937207078581E-01 3.118897307111E+00
H 1.056754871225E+01 -2.089190202808E-01 3.211520795099E+00
H 3.677469452753E+00 -1.191108299090E+00 2.989778251681E+00
H -3.212609806747E+00 -2.056703598645E+00 2.475375381979E+00
H -1.010268906625E+01 -2.720974420068E+00 1.718665522934E+00
H -1.699276832575E+01 -3.118897307111E+00 7.937207078581E-01
H 2.205101414475E+01 -3.211520795099E+00 -2.089190202808E-01
H 1.516093488525E+01 -2.989778251681E+00 -1.191108299090E+00
H 8.270855625753E+00 -2.475375381979E+00 -2.056703598645E+00
H 1.380776366253E+00 -1.718665522934E+00 -2.720974420068E+00
H -5.509302893247E+00 -7.937207078581E-01 -3.118897307111E+00
H -1.239938215275E+01 2.089190202808E-01 -3.211520795099E+00
H -1.928946141225E+01 1.191108299090E+00 -2.989778251681E+00
H 1.975432105825E+01 2.056703598645E+00 -2.475375381979E+00
H 1.286424179875E+01 2.720974420068E+00 -1.718665522934E+00
H 5.974162539253E+00 3.118897307111E+00 -7.937207078581E-01
H -1.370149547048E+00 2.489875675527E+00 1.763702758053E+00
H -8.260228806548E+00 1.822998360710E+00 2.446794898473E+00
H -1.515030806605E+01 9.776732647710E-01 2.890377706407E+00
H -2.204038732555E+01 3.664669782569E-02 3.051030205993E+00
H 1.700339514495E+01 -9.079671032354E-01 2.913026611239E+00
H 1.011331588545E+01 -1.763702758053E+00 2.489875675527E+00
H 3.223236625952E+00 -2.446794898473E+00 1.822998360710E+00
H -3.666842633548E+00 -2.890377706407E+00 9.776732647710E-01
H -1.055692189305E+01 -3.051030205993E+00 3.664669782569E-02
H -1.744700115255E+01 -2.913026611239E+00 -9.079671032354E-01
H 2.159678131795E+01 -2.489875675527E+00 -1.763702758053E+00
H 1.470670205845E+01 -1.822998360710E+00 -2.446794898473E+00
H 7.816622798952E+00 -9.776732647710E-01 -2.890377706407E+00
H 9.265435394521E-01 -3.664669782569E-02 -3.051030205993E+00
H -5.963535720048E+00 9.079671032354E-01 -2.913026611239E+00

H -1.285361497955E+01 1.763702758053E+00 -2.489875675527E+00
H -1.974369423905E+01 2.446794898473E+00 -1.822998360710E+00
H 1.930008823145E+01 2.890377706407E+00 -9.776732647710E-01
H 1.241000897195E+01 3.051030205993E+00 -3.664669782569E-02
H 5.519929712452E+00 2.913026611239E+00 9.079671032354E-01

PbE0/POB-TZVP optimized geometry, *all*-[106.2]-$(PbMe_2)_\infty$

Energy (a.u): -8.1781968463725E+02
Unit cell length (Å): 6.75406230

Pb	-2.059635330313E+00	1.028192106855E+00	-3.247134024684E-01
Pb	1.917187696866E-01	-2.328859979406E-01	1.052797185741E+00
Pb	2.443072869687E+00	-7.953061089144E-01	-7.280837832729E-01
C	-1.552968041595E+00	1.819954464414E+00	-2.369181938950E+00
C	6.983860584049E-01	1.141794513111E+00	2.760717769388E+00
C	2.949740158405E+00	-2.961748977525E+00	-3.915358304384E-01
C	-2.905742962237E+00	2.797372861110E+00	7.805953646797E-01
C	-6.543888622369E-01	-2.074701846444E+00	2.032298279239E+00
C	1.596965237763E+00	-7.226710146660E-01	-2.812893643918E+00
H	-1.255975585869E+00	1.004934704668E+00	-3.025537768097E+00
H	9.953785141309E-01	2.117725214947E+00	2.383067867436E+00
H	3.246732614131E+00	-3.122659919615E+00	6.424699006614E-01
H	-7.313940292204E-01	2.530938162541E+00	-2.294197564933E+00
H	1.519960070780E+00	7.213642912619E-01	3.338955526635E+00
H	-2.982748129220E+00	-3.252302453803E+00	-1.044757961702E+00
H	-2.417231525970E+00	2.323719877517E+00	-2.798396528109E+00
H	-1.658774259702E-01	1.261622544446E+00	3.411598709263E+00
H	2.085476674030E+00	-3.585342421963E+00	-6.132021811541E-01
H	2.997718019686E+00	3.198021449765E+00	2.314164072407E-01
H	-1.504990180314E+00	-1.799423212405E+00	2.653859613724E+00
H	7.463639196862E-01	-1.398598237360E+00	-2.885276020964E+00
H	-2.149206393480E+00	3.574611573838E+00	8.758206339167E-01
H	1.021477065200E-01	-2.545788705049E+00	2.657794114647E+00
H	2.353501806520E+00	-1.028822868789E+00	-3.533614748564E+00
H	-3.232018542888E+00	2.499169252157E+00	1.774480342929E+00
H	-9.806644428880E-01	-2.786329681571E+00	1.277103889260E+00
H	1.270689657112E+00	2.871604294141E-01	-3.051584232189E+00

PbE0/POB-TZVP optimized geometry, *all*-[-93.9]-$(PbMe_2)_\infty$

Energy (a.u): -4.3617001685785E+03
Unit cell length (Å): 33.59883904

Pb	-2.535122702406E+00	1.177587304319E+00	-3.617337474224E-01
Pb	3.764659617594E+00	1.226378320271E+00	1.164447460642E-01
Pb	1.006444193759E+01	1.088464354110E+00	5.768955825368E-01
Pb	1.636422425759E+01	7.848415569885E-01	9.495192961396E-01
Pb	-1.093483246241E+01	3.617337474224E-01	1.177587304319E+00
Pb	-4.635050142406E+00	-1.164447460642E-01	1.226378320271E+00
Pb	1.664732177594E+00	-5.768955825368E-01	1.088464354110E+00
Pb	7.964514497594E+00	-9.495192961396E-01	7.848415569885E-01
Pb	1.426429681759E+01	-1.177587304319E+00	3.617337474224E-01
Pb	-1.303475990241E+01	-1.226378320271E+00	-1.164447460642E-01
Pb	-6.734977582406E+00	-1.088464354110E+00	-5.768955825368E-01
Pb	-4.351952624062E-01	-7.848415569885E-01	-9.495192961396E-01
Pb	5.864587057594E+00	-3.617337474224E-01	-1.177587304319E+00
Pb	1.216436937759E+01	1.164447460642E-01	-1.226378320271E+00
Pb	-1.513468734241E+01	5.768955825368E-01	-1.088464354110E+00
Pb	-8.834905022406E+00	9.495192961396E-01	-7.848415569885E-01
C	-3.114811297508E+00	1.989745466642E+00	-2.379885780827E+00
C	3.184971022492E+00	2.749027970781E+00	-1.437285137913E+00
C	9.484753342492E+00	3.089795886370E+00	-2.758708617745E-01
C	1.578453566249E+01	2.960170387328E+00	9.275422522939E-01
C	-1.151452105751E+01	2.379885780827E+00	1.989745466642E+00
C	-5.214738737508E+00	1.437285137913E+00	2.749027970781E+00
C	1.085043582492E+00	2.758708617745E-01	3.089795886370E+00
C	7.384825902492E+00	-9.275422522939E-01	2.960170387328E+00
C	1.368460822249E+01	-1.989745466642E+00	2.379885780827E+00
C	-1.361444849751E+01	-2.749027970781E+00	1.437285137913E+00
C	-7.314666177508E+00	-3.089795886370E+00	2.758708617745E-01
C	-1.014883857508E+00	-2.960170387328E+00	-9.275422522939E-01
C	5.284898462492E+00	-2.379885780827E+00	-1.989745466642E+00
C	1.158468078249E+01	-1.437285137913E+00	-2.749027970781E+00
C	-1.571437593751E+01	-2.758708617745E-01	-3.089795886370E+00
C	-9.414593617508E+00	9.275422522939E-01	-2.960170387328E+00
C	-1.363579138733E+00	2.858910031337E+00	5.747516967564E-01
C	4.936203181267E+00	2.421340511171E+00	1.625058832524E+00
C	1.123598550127E+01	1.615143847686E+00	2.427965492236E+00
C	-1.606307121873E+01	5.630561747057E-01	2.861236415316E+00
C	-9.763288898733E+00	-5.747516967564E-01	2.858910031337E+00
C	-3.463506578733E+00	-1.625058832524E+00	2.421340511171E+00
C	2.836275741268E+00	-2.427965492236E+00	1.615143847686E+00
C	9.136058061268E+00	-2.861236415316E+00	5.630561747057E-01

C 1.543584038127E+01 -2.858910031337E+00 -5.747516967564E-01
C -1.186321633873E+01 -2.421340511171E+00 -1.625058832524E+00
C -5.563434018733E+00 -1.615143847686E+00 -2.427965492236E+00
C 7.363483012675E-01 -5.630561747057E-01 -2.861236415316E+00
C 7.036130621268E+00 5.747516967564E-01 -2.858910031337E+00
C 1.333591294127E+01 1.625058832524E+00 -2.421340511171E+00
C -1.396314377873E+01 2.427965492236E+00 -1.615143847686E+00
C -7.663361458733E+00 2.861236415316E+00 -5.630561747057E-01
H -3.474477458705E+00 1.191743515677E+00 -3.025808952476E+00
H 2.825304861295E+00 2.258954397752E+00 -2.339422461404E+00
H 9.125087181295E+00 2.982259950241E+00 -1.296880107500E+00
H 1.542486950130E+01 3.251543459560E+00 -5.689951347751E-02
H -1.187418721870E+01 3.025808952476E+00 1.191743515677E+00
H -5.574404898705E+00 2.339422461404E+00 2.258954397752E+00
H 7.253774212951E-01 1.296880107500E+00 2.982259950241E+00
H 7.025159741295E+00 5.689951347751E-02 3.251543459560E+00
H 1.332494206130E+01 -1.191743515677E+00 3.025808952476E+00
H -1.397411465870E+01 -2.258954397752E+00 2.339422461404E+00
H -7.674332338705E+00 -2.982259950241E+00 1.296880107500E+00
H -1.374550018705E+00 -3.251543459560E+00 5.689951347751E-02
H 4.925232301295E+00 -3.025808952476E+00 -1.191743515677E+00
H 1.122501462130E+01 -2.339422461404E+00 -2.258954397752E+00
H -1.607404209870E+01 -1.296880107500E+00 -2.982259950241E+00
H -9.774259778705E+00 -5.689951347751E-02 -3.251543459560E+00
H -2.254550358936E+00 2.463430407366E+00 -2.849162957547E+00
H 4.045231961064E+00 3.366240393093E+00 -1.689569337584E+00
H 1.034501428106E+01 3.756570794017E+00 -2.727541019574E-01
H 1.664479660106E+01 3.574997344950E+00 1.185585473170E+00
H -1.065426011894E+01 2.849162957547E+00 2.463430407366E+00
H -4.354477798936E+00 1.689569337584E+00 3.366240393093E+00
H 1.945304521064E+00 2.727541019574E-01 3.756570794017E+00
H 8.245086841064E+00 -1.185585473170E+00 3.574997344950E+00
H 1.454486916106E+01 -2.463430407366E+00 2.849162957547E+00
H -1.275418755894E+01 -3.366240393093E+00 1.689569337584E+00
H -6.454405238936E+00 -3.756570794017E+00 2.727541019574E-01
H -1.546229189357E-01 -3.574997344950E+00 -1.185585473170E+00
H 6.145159401064E+00 -2.849162957547E+00 -2.463430407366E+00
H 1.244494172106E+01 -1.689569337584E+00 -3.366240393093E+00
H -1.485411499894E+01 -2.727541019574E-01 -3.756570794017E+00
H -8.554332678936E+00 1.185585473170E+00 -3.574997344950E+00
H -3.904836889546E+00 2.730508487395E+00 -2.263249152512E+00
H 2.394945430454E+00 3.388768858833E+00 -1.046049208921E+00
H 8.694727750454E+00 3.531119890780E+00 3.304022442685E-01
H 1.499451007045E+01 3.135889929038E+00 1.656552950872E+00
H -1.230454664955E+01 2.263249152512E+00 2.730508487395E+00

H -6.004764329546E+00 1.046049208921E+00 3.388768858833E+00
H 2.950179904539E-01 -3.304022442685E-01 3.531119890780E+00
H 6.594800310454E+00 -1.656552950872E+00 3.135889929038E+00
H 1.289458263045E+01 -2.730508487395E+00 2.263249152512E+00
H -1.440447408955E+01 -3.388768858833E+00 1.046049208921E+00
H -8.104691769546E+00 -3.531119890780E+00 -3.304022442685E-01
H -1.804909449546E+00 -3.135889929038E+00 -1.656552950872E+00
H 4.494872870454E+00 -2.263249152512E+00 -2.730508487395E+00
H 1.079465519045E+01 -1.046049208921E+00 -3.388768858833E+00
H -1.650440152955E+01 3.304022442685E-01 -3.531119890780E+00
H -1.020461920955E+01 1.656552950872E+00 -3.135889929038E+00
H -2.013814891026E+00 3.716070796575E+00 7.431171355700E-01
H 4.285967428974E+00 3.148823134229E+00 2.108629439157E+00
H 1.058574974897E+01 2.102195693850E+00 3.153122025405E+00
H -1.671330697103E+01 7.355280155335E-01 3.717580366408E+00
H -1.041352465103E+01 -7.431171355700E-01 3.716070796575E+00
H -4.113742331026E+00 -2.108629439157E+00 3.148823134229E+00
H 2.186039988974E+00 -3.153122025405E+00 2.102195693850E+00
H 8.485822308974E+00 -3.717580366408E+00 7.355280155335E-01
H 1.478560462897E+01 -3.716070796575E+00 -7.431171355700E-01
H -1.251345209103E+01 -3.148823134229E+00 -2.108629439157E+00
H -6.213669771026E+00 -2.102195693850E+00 -3.153122025405E+00
H 8.611254897434E-02 -7.355280155335E-01 -3.717580366408E+00
H 6.385894868974E+00 7.431171355700E-01 -3.716070796575E+00
H 1.268567718897E+01 2.108629439157E+00 -3.148823134229E+00
H -1.461337953103E+01 3.153122025405E+00 -2.102195693850E+00
H -8.313597211026E+00 3.717580366408E+00 -7.355280155335E-01
H -5.563639159429E-01 3.154319828675E+00 -9.372054978403E-02
H 5.743418404057E+00 2.950076830382E+00 1.120519441093E+00
H 1.204320072406E+01 2.296711377176E+00 2.164170504598E+00
H -1.525585599594E+01 1.293692436536E+00 2.878346227033E+00
H -8.956073675943E+00 9.372054978403E-02 3.154319828675E+00
H -2.656291355943E+00 -1.120519441093E+00 2.950076830382E+00
H 3.643490964057E+00 -2.164170504598E+00 2.296711377176E+00
H 9.943273284057E+00 -2.878346227033E+00 1.293692436536E+00
H 1.624305560406E+01 -3.154319828675E+00 9.372054978403E-02
H -1.105600111594E+01 -2.950076830382E+00 -1.120519441093E+00
H -4.756218795943E+00 -2.296711377176E+00 -2.164170504598E+00
H 1.543563524057E+00 -1.293692436536E+00 -2.878346227033E+00
H 7.843345844057E+00 -9.372054978403E-02 -3.154319828675E+00
H 1.414312816406E+01 1.120519441093E+00 -2.950076830382E+00
H -1.315592855594E+01 2.164170504598E+00 -2.296711377176E+00
H -6.856146235943E+00 2.878346227033E+00 -1.293692436536E+00
H -9.428390392168E-01 2.545339055994E+00 1.527631531523E+00
H 5.356943280783E+00 1.766987379262E+00 2.385406591674E+00

H 1.165672560078E+01 7.196278918180E-01 2.880025122007E+00
H -1.564233111922E+01 -4.372884187123E-01 2.936185935007E+00
H -9.342548799217E+00 -1.527631531523E+00 2.545339055994E+00
H -3.042766479217E+00 -2.385406591674E+00 1.766987379262E+00
H 3.257015840783E+00 -2.880025122007E+00 7.196278918180E-01
H 9.556798160783E+00 -2.936185935007E+00 -4.372884187123E-01
H 1.585658048078E+01 -2.545339055994E+00 -1.527631531523E+00
H -1.144247623922E+01 -1.766987379262E+00 -2.385406591674E+00
H -5.142693919217E+00 -7.196278918180E-01 -2.880025122007E+00
H 1.157088400783E+00 4.372884187123E-01 -2.936185935007E+00
H 7.456870720783E+00 1.527631531523E+00 -2.545339055994E+00
H 1.375665304078E+01 2.385406591674E+00 -1.766987379262E+00
H -1.354240367922E+01 2.880025122007E+00 -7.196278918180E-01
H -7.242621359217E+00 2.936185935007E+00 4.372884187123E-01

PbE0/POB-TZVP optimized geometry, *all*-[-85.3]-$(PbMe_2)_\infty$

Energy (a.u): -2.7260673370996E+03
Unit cell length (Å): 19.72652919

Pb	-1.258232181336E-01	1.301536642341E+00	-3.642430760127E-01
Pb	1.741767818664E-01	1.267061970785E+00	4.703452051086E-01
Pb	4.741767818664E-01	7.486126922423E-01	1.125277604324E+00
Pb	-2.258232181336E-01	-5.578119032781E-02	1.350392205467E+00
Pb	7.417678186640E-02	-8.388685541257E-01	1.059702882264E+00
Pb	3.741767818664E-01	-1.301536642341E+00	3.642430760127E-01
Pb	-3.258232181336E-01	-1.267061970785E+00	-4.703452051086E-01
Pb	-2.582321813360E-02	-7.486126922423E-01	-1.125277604324E+00
Pb	2.741767818664E-01	5.578119032781E-02	-1.350392205467E+00
Pb	-4.258232181336E-01	8.388685541257E-01	-1.059702882264E+00
C	-1.589882301652E-01	2.168909188524E+00	-2.337144070644E+00
C	1.410117698348E-01	3.128423209979E+00	-6.159364368776E-01
C	4.410117698348E-01	2.892985896416E+00	1.340537980867E+00
C	-2.589882301652E-01	1.552526299397E+00	2.784972453130E+00
C	4.101176983480E-02	-3.809455755646E-01	3.165642106030E+00
C	3.410117698348E-01	-2.168909188524E+00	2.337144070644E+00
C	-3.589882301652E-01	-3.128423209979E+00	6.159364368776E-01
C	-5.898823016520E-02	-2.892985896416E+00	-1.340537980867E+00
C	2.410117698348E-01	-1.552526299397E+00	-2.784972453130E+00
C	-4.589882301652E-01	3.809455755646E-01	-3.165642106030E+00
C	-5.578639050585E-02	2.875397712917E+00	4.731578768453E-01
C	2.442136094942E-01	2.048130393321E+00	2.072909133518E+00
C	-4.557863905059E-01	4.385468768681E-01	2.880879556777E+00
C	-1.557863905059E-01	-1.338546640888E+00	2.588451906842E+00
C	1.442136094941E-01	-2.604360837352E+00	1.307323606738E+00
C	4.442136094941E-01	-2.875397712917E+00	-4.731578768453E-01
C	-2.557863905058E-01	-2.048130393321E+00	-2.072909133518E+00
C	4.421360949415E-02	-4.385468768681E-01	-2.880879556777E+00
C	3.442136094942E-01	1.338546640888E+00	-2.588451906842E+00
C	-3.557863905059E-01	2.604360837352E+00	-1.307323606738E+00
H	-1.853101565329E-01	1.419843369540E+00	-2.931844889823E+00
H	1.146898434671E-01	2.871972603555E+00	-1.537349347557E+00
H	4.146898434671E-01	3.227105917771E+00	4.443613928928E-01
H	-2.853101565329E-01	2.349594456694E+00	2.256341184546E+00
H	1.468984346710E-02	5.746177729386E-01	3.206475333919E+00
H	3.146898434671E-01	-1.419843369540E+00	2.931844889823E+00
H	-3.853101565329E-01	-2.871972603555E+00	1.537349347557E+00
H	-8.531015653290E-02	-3.227105917771E+00	-4.443613928928E-01
H	2.146898434671E-01	-2.349594456694E+00	-2.256341184546E+00
H	-4.853101565329E-01	-5.746177729386E-01	-3.206475333919E+00

H -1.151645724498E-01 2.525842214152E+00 -2.893847252320E+00
H 1.848354275502E-01 3.744410013659E+00 -8.565188031558E-01
H 4.848354275502E-01 3.532740455764E+00 1.507970716811E+00
H -2.151645724498E-01 1.971684117199E+00 3.296466676995E+00
H 8.483542755020E-02 -3.424885390578E-01 3.825824409348E+00
H 3.848354275502E-01 -2.525842214152E+00 2.893847252320E+00
H -3.151645724498E-01 -3.744410013659E+00 8.565188031558E-01
H -1.516457244980E-02 -3.532740455764E+00 -1.507970716811E+00
H 2.848354275502E-01 -1.971684117199E+00 -3.296466676995E+00
H -4.151645724498E-01 3.424885390578E-01 -3.825824409348E+00
H -1.931543882689E-01 3.005114487534E+00 -2.155803426366E+00
H 1.068456117311E-01 3.698338151317E+00 2.228036876110E-02
H 4.068456117311E-01 2.978922343187E+00 2.191853820303E+00
H -2.931543882689E-01 1.121659449806E+00 3.524213610861E+00
H 6.845611731100E-03 -1.164039229598E+00 3.510443585685E+00
H 3.068456117311E-01 -3.005114487534E+00 2.155803426366E+00
H -3.931543882689E-01 -3.698338151317E+00 -2.228036876110E-02
H -9.315438826890E-02 -2.978922343187E+00 -2.191853820303E+00
H 2.068456117311E-01 -1.121659449806E+00 -3.524213610861E+00
H -4.931543882689E-01 1.164039229598E+00 -3.510443585685E+00
H -8.466094429607E-02 3.753175557093E+00 7.749192260872E-01
H 2.153390557039E-01 2.580896715749E+00 2.832984064896E+00
H -4.846609442961E-01 4.228030504418E-01 3.808945280502E+00
H -1.846609442961E-01 -1.896787009587E+00 3.330018860244E+00
H 1.153390557039E-01 -3.491868901373E+00 1.579138418551E+00
H 4.153390557039E-01 -3.753175557093E+00 -7.749192260872E-01
H -2.846609442961E-01 -2.580896715749E+00 -2.832984064896E+00
H 1.533905570393E-02 -4.228030504418E-01 -3.808945280502E+00
H 3.153390557039E-01 1.896787009587E+00 -3.330018860244E+00
H -3.846609442961E-01 3.491868901373E+00 -1.579138418551E+00
H -1.937556617607E-02 3.163478404523E+00 -2.923327145486E-01
H 2.806244338239E-01 2.731136648972E+00 1.622943818043E+00
H -4.193755661761E-01 1.255593521433E+00 2.918310973973E+00
H -1.193755661761E-01 -6.995436552381E-01 3.098982527588E+00
H 1.806244338239E-01 -2.387478932223E+00 2.095948086206E+00
H 4.806244338239E-01 -3.163478404523E+00 2.923327145486E-01
H -2.193755661761E-01 -2.731136648972E+00 -1.622943818043E+00
H 8.062443382393E-02 -1.255593521433E+00 -2.918310973973E+00
H 3.806244338239E-01 6.995436552381E-01 -3.098982527588E+00
H -3.193755661761E-01 2.387478932223E+00 -2.095948086206E+00
H -2.883945347158E-02 2.486647074541E+00 1.339683940616E+00
H 2.711605465284E-01 1.224293279289E+00 2.545441553121E+00
H -4.288394534716E-01 -5.056989364529E-01 2.778927008710E+00
H -1.288394534716E-01 -2.042531346545E+00 1.950956799227E+00
H 1.711605465284E-01 -2.799186205344E+00 3.777874030219E-01

H 4.711605465284E-01 -2.486647074541E+00 -1.339683940616E+00
H -2.288394534716E-01 -1.224293279289E+00 -2.545441553121E+00
H 7.116054652842E-02 5.056989364529E-01 -2.778927008710E+00
H 3.711605465284E-01 2.042531346545E+00 -1.950956799227E+00
H -3.288394534716E-01 2.799186205344E+00 -3.777874030219E-01

PbE0/POB-TZVP optimized geometry, *all*-[61.1]-$(PbMe_2)_\infty$

Energy (a.u): -1.0086435406771E+04
Unit cell length (Å): 66.59830526

Pb	4.649444067342E-01	2.214964331952E-01	1.647143902578E+00
Pb	-6.734872378131E+00	-6.005826208136E-02	1.660884315921E+00
Pb	-1.393468916300E+01	-3.398851905056E-01	1.626844111460E+00
Pb	-2.113450594786E+01	-6.099342408265E-01	1.546002563900E+00
Pb	-2.833432273273E+01	-8.624365935432E-01	1.420685337376E+00
Pb	3.106416574241E+01	-1.090128215698E+00	1.254497580331E+00
Pb	2.386434895755E+01	-1.286458833879E+00	1.052220211958E+00
Pb	1.666453217268E+01	-1.445780373658E+00	8.196723838597E-01
Pb	9.464715387815E+00	-1.563509444414E+00	5.635440736512E-01
Pb	2.264898602950E+00	-1.636259195128E+00	2.912036264860E-01
Pb	-4.934918181914E+00	-1.661936747927E+00	1.048578117979E-02
Pb	-1.213473496678E+01	-1.639803406370E+00	-2.705337209595E-01
Pb	-1.933455175164E+01	-1.570495906394E+00	-5.437704605063E-01
Pb	-2.653436853651E+01	-1.456008098585E+00	-8.013639139447E-01
Pb	3.286411993863E+01	-1.299633588728E+00	-1.035903586619E+00
Pb	2.566430315376E+01	-1.105870986759E+00	-1.240642199170E+00
Pb	1.846448636890E+01	-8.802944899562E-01	-1.409689794483E+00
Pb	1.126466958403E+01	-6.293935234252E-01	-1.538183181025E+00
Pb	4.064852799167E+00	-3.603860511592E-01	-1.622425838012E+00
Pb	-3.134963985698E+00	-8.101092835450E-02	-1.659994257582E+00
Pb	-1.033478077056E+01	2.006947313627E-01	-1.649807664706E+00
Pb	-1.753459755543E+01	4.766267690625E-01	-1.592159109113E+00
Pb	-2.473441434029E+01	7.388471224086E-01	-1.488707034788E+00
Pb	-3.193423112516E+01	9.798121892586E-01	-1.342427569554E+00
Pb	2.746425734998E+01	1.192589843363E+00	-1.157528907296E+00
Pb	2.026444056511E+01	1.371058859017E+00	-9.393302458821E-01
Pb	1.306462378025E+01	1.510085007578E+00	-6.941087635288E-01
Pb	5.864806995383E+00	1.605668759875E+00	-4.289190358094E-01
Pb	-1.335009789482E+00	1.655060345384E+00	-1.513900883607E-01
Pb	-8.534826574347E+00	1.656838858118E+00	1.304940762948E-01
Pb	-1.573464335921E+01	1.610953133503E+00	4.086241639654E-01
Pb	-2.293446014408E+01	1.518723220291E+00	6.749988784188E-01
Pb	-3.013427692894E+01	1.382802405164E+00	9.219551041075E-01
Pb	2.926421154619E+01	1.207100882503E+00	1.142388360050E+00
Pb	2.206439476133E+01	9.966732652150E-01	1.329957182816E+00
Pb	1.486457797646E+01	7.575731727253E-01	1.479265558879E+00
Pb	7.664761191599E+00	4.966790793663E-01	1.586018158105E+00
C	1.843474752709E+00	1.602816964837E+00	2.775188795540E+00
C	-5.356342032156E+00	1.110752718924E+00	3.006147612986E+00
C	-1.255615881702E+01	5.867341396305E-01	3.150625036886E+00

C -1.975597560189E+01 4.583628740377E-02 3.204464714803E+00
C -2.695579238675E+01 -4.963801913577E-01 3.166117777229E+00
C 3.244269608838E+01 -1.024316715771E+00 3.036687395741E+00
C 2.524287930352E+01 -1.522785513240E+00 2.819897046760E+00
C 1.804306251866E+01 -1.977446544022E+00 2.521983393917E+00
C 1.084324573379E+01 -2.375220038060E+00 2.151516870595E+00
C 3.643428948925E+00 -2.704662776156E+00 1.719155124163E+00
C -3.556387835939E+00 -2.956297290549E+00 1.237336414867E+00
C -1.075620462080E+01 -3.122884514409E+00 7.199217897272E-01
C -1.795602140567E+01 -3.199632036612E+00 1.817963254556E-01
C -2.515583819053E+01 -3.184331970676E+00 -3.615590881036E-01
C -3.235565497540E+01 -3.077424471643E+00 -8.945131049871E-01
C 2.704283349974E+01 -2.881985073613E+00 -1.401733608476E+00
C 1.984301671487E+01 -2.603636212233E+00 -1.868628788179E+00
C 1.264319993001E+01 -2.250385477455E+00 -2.281766919850E+00
C 5.443383145141E+00 -1.832395249757E+00 -2.629262771639E+00
C -1.756433639723E+00 -1.361690346957E+00 -2.901119520575E+00
C -8.956250424588E+00 -8.518120920988E-01 -3.089516342960E+00
C -1.615606720945E+01 -3.174287542412E-01 -3.189033405225E+00
C -2.335588399432E+01 2.260864309348E-01 -3.196807782681E+00
C -3.055570077918E+01 7.630975211273E-01 -3.112615820642E+00
C 2.884278769595E+01 1.278155685005E+00 -2.938879568568E+00
C 2.164297091109E+01 1.756443636958E+00 -2.680597102112E+00
C 1.444315412622E+01 2.184201903424E+00 -2.345198737579E+00
C 7.243337341358E+00 2.549124657895E+00 -1.942333275258E+00
C 4.352055649287E-02 2.840713737138E+00 -1.483590421005E+00
C -7.156296228372E+00 3.050580654238E+00 -9.821673715060E-01
C -1.435611301324E+01 3.172687920093E+00 -4.524891549565E-01
C -2.155592979810E+01 3.203522730986E+00 9.020635073607E-02
C -2.875574658297E+01 3.142198025548E+00 6.303067839563E-01
C 3.064274189217E+01 2.990478003900E+00 1.152274438599E+00
C 2.344292510730E+01 2.752727374830E+00 1.641093255583E+00
C 1.624310832244E+01 2.435785791064E+00 2.082700807536E+00
C 9.043291537574E+00 2.048771084913E+00 2.464392849220E+00
C -5.340997498021E-01 -1.029332064951E+00 3.232102654802E+00
C -7.733916534667E+00 -1.560754060273E+00 3.011653837090E+00
C -1.493373331953E+01 -2.047276002938E+00 2.704565221789E+00
C -2.213355010440E+01 -2.474901542465E+00 2.319671189246E+00
C -2.933336688926E+01 -2.831328670657E+00 1.868044440004E+00
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H 3.147165505542E+01 -5.302697615410E-01 -3.363365891497E+00
H 2.427183827056E+01 4.576928095447E-02 -3.404602959673E+00
H 1.707202148569E+01 6.204916245688E-01 -3.347895799444E+00
H 9.872204700830E+00 1.177363553871E+00 -3.194875772563E+00
H 2.672387915965E+00 1.700364877348E+00 -2.949944986601E+00
H -4.527428868900E+00 2.174449799150E+00 -2.620149654326E+00
H -1.172724565376E+01 2.585979759242E+00 -2.214977386991E+00
H -1.892706243863E+01 2.923115789942E+00 -1.746084253031E+00
H -2.612687922349E+01 3.176159101469E+00 -1.226959454199E+00
H 3.327160925164E+01 3.337830098465E+00 -6.725372657893E-01
H 2.607179246678E+01 3.403477800700E+00 -9.876740472814E-02
H 1.887197568191E+01 3.371213643305E+00 4.778438147417E-01
H 1.167215889705E+01 3.241965807346E+00 1.040708337669E+00
H 4.472342112181E+00 3.019452517741E+00 1.573633576535E+00
H -2.727474672683E+00 2.710075076705E+00 2.061288242512E+00
H -9.927291457548E+00 2.322733709933E+00 2.489643398729E+00
H -1.712710824241E+01 1.868571523317E+00 2.846376047247E+00
H -2.432692502728E+01 1.360653936074E+00 3.121223639270E+00
H -3.152674181214E+01 8.135928124273E-01 3.306279309989E+00
H 2.787174666299E+01 2.431261048717E-01 3.396219344686E+00
H 2.067192987813E+01 -3.343348980626E-01 3.388456332319E+00
H 1.347211309326E+01 -9.021776947015E-01 3.283213600617E+00
H 6.272296308397E+00 -1.444066481655E+00 3.083518791357E+00

PbE0/POB-TZVP optimized geometry, *all*-[-50.4]-$(PbMe_2)_\infty$

Energy (a.u): -8.4508170244107E+03
Unit cell length (Å): 49.91442606

Pb	9.429104615514E-03	-4.544177041764E-01	1.828368410210E+00
Pb	-2.808934760296E-01	-8.131636022281E-01	1.699467990088E+00
Pb	4.287839433252E-01	-1.138618486862E+00	1.500991150773E+00
Pb	1.384613626800E-01	-1.417458196862E+00	1.241063557386E+00
Pb	-1.518612179651E-01	-1.638267001738E+00	9.303266761414E-01
Pb	-4.421837986103E-01	-1.792004963074E+00	5.815021114666E-01
Pb	2.674936207445E-01	-1.872378030671E+00	2.088707820247E-01
Pb	-2.282895990061E-02	-1.876095721697E+00	-1.723117417746E-01
Pb	-3.131515405458E-01	-1.803005833445E+00	-5.464398026198E-01
Pb	3.965258788091E-01	-1.656100674527E+00	-8.981965537419E-01
Pb	1.062032981639E-01	-1.441394559411E+00	-1.213181032420E+00
Pb	-1.841192824813E-01	-1.167677581675E+00	-1.478497737088E+00
Pb	-4.744418631264E-01	-8.461557465501E-01	-1.683284570684E+00
Pb	2.352355562284E-01	-4.899921957419E-01	-1.819157536178E+00
Pb	-5.508702441674E-02	-1.137683068684E-01	-1.880553978400E+00
Pb	-3.454096050619E-01	2.671132698555E-01	-1.864960319790E+00
Pb	3.642678142929E-01	6.370591979270E-01	-1.773014966564E+00
Pb	7.394523364777E-02	9.809238475842E-01	-1.608482172286E+00
Pb	-2.163773469974E-01	1.284629359668E+00	-1.378097928887E+00
Pb	4.933000723575E-01	1.535741994829E+00	-1.091294194359E+00
Pb	2.029774917123E-01	1.723981172279E+00	-7.598127472931E-01
Pb	-8.734508893287E-02	1.841640357978E+00	-3.972244770783E-01
Pb	-3.776676695780E-01	1.883902571037E+00	-1.837379010010E-02
Pb	3.320097497768E-01	1.849037591489E+00	3.612291220036E-01
Pb	4.168716913165E-02	1.738472795693E+00	7.260432714099E-01
Pb	-2.486354115135E-01	1.556734719379E+00	1.061133123978E+00
Pb	4.610420078413E-01	1.311263740745E+00	1.352780061773E+00
Pb	1.707194271962E-01	1.012109470498E+00	1.589044024894E+00
Pb	-1.196031534490E-01	6.715193196110E-01	1.760252338931E+00
Pb	-4.099257340942E-01	3.034370888791E-01	1.859395715391E+00
Pb	2.997516852607E-01	-7.706789192387E-02	1.882415212794E+00
C	4.166493235802E-02	-1.686517750387E+00	2.819737840289E+00
C	-2.486576482871E-01	-2.219603687246E+00	2.422524113790E+00
C	4.610197710677E-01	-2.661818788357E+00	1.926131965437E+00
C	1.706971904225E-01	-2.995058715522E+00	1.350883748109E+00
C	-1.196253902226E-01	-3.205680586969E+00	7.203301914107E-01
C	-4.099479708678E-01	-3.285061518534E+00	6.028623204106E-02
C	2.997294484871E-01	-3.229951645552E+00	-6.022258527516E-01
C	9.406867841892E-03	-3.042607172698E+00	-1.240082740374E+00
C	-2.809157128033E-01	-2.730698004703E+00	-1.827170494902E+00

C 4.287617065516E-01 -2.306993739551E+00 -2.339453674686E+00
C 1.384391259064E-01 -1.788840879642E+00 -2.755959346153E+00
C -1.518834547388E-01 -1.197452663941E+00 -3.059635718178E+00
C -4.422060353839E-01 -5.570405954831E-01 -3.238050244408E+00
C 2.674713839709E-01 1.061767804032E-01 -3.283898613178E+00
C -2.285119667424E-02 7.650472664247E-01 -3.195303786882E+00
C -3.131737773194E-01 1.392596627469E+00 -2.975892848120E+00
C 3.965036420354E-01 1.963132918962E+00 -2.634648506502E+00
C 1.061810613903E-01 2.453298318095E+00 -2.185541345471E+00
C -1.841415192549E-01 2.843025395834E+00 -1.646957864965E+00
C -4.744640999000E-01 3.116358679827E+00 -1.040947735959E+00
C 2.352133194548E-01 3.262107873310E+00 -3.923210843361E-01
C -5.510926119036E-02 3.274305987179E+00 2.723672385751E-01
C -3.454318418355E-01 3.152453629219E+00 9.259048147372E-01
C 3.642455775193E-01 2.901539449280E+00 1.541535738995E+00
C 7.392299687415E-02 2.531835903372E+00 2.094056008975E+00
C -2.163995837710E-01 2.058478698101E+00 2.560845379907E+00
C 4.932778355838E-01 1.500847133070E+00 2.922793440099E+00
C 2.029552549387E-01 8.817707100679E-01 3.165081993439E+00
C -8.736732570650E-02 2.265944905924E-01 3.277791718087E+00
C -3.776899063517E-01 -4.378585339518E-01 3.256308264672E+00
C 3.319875130032E-01 -1.084385578670E+00 3.101511168302E+00
C -1.154750091852E-02 5.941837172003E-01 3.527599312787E+00
C -3.018700815637E-01 -1.280797795274E-01 3.574997450550E+00
C 4.078073377912E-01 -8.450996750325E-01 3.476034772643E+00
C 1.174847571460E-01 -1.527521090547E+00 3.234762822727E+00
C -1.728378234992E-01 -2.147405613138E+00 2.861059302780E+00
C -4.631604041443E-01 -2.679375097618E+00 2.370223678817E+00
C 2.465170152105E-01 -3.101650650788E+00 1.782350818954E+00
C -4.380556543465E-02 -3.396944261887E+00 1.121508307146E+00
C -3.341281460798E-01 -3.553166575779E+00 4.147511134715E-01
C 3.755492732750E-01 -3.563921832580E+00 -3.089860395197E-01
C 8.522669262987E-02 -3.428769710813E+00 -1.020073267749E+00
C -2.050958880153E-01 -3.153243354221E+00 -1.689398576542E+00
C -4.954184686605E-01 -2.748622844217E+00 -2.289559709117E+00
C 2.142589506944E-01 -2.231473392021E+00 -2.795985998188E+00
C -7.606362995078E-02 -1.622967156969E+00 -3.187944291979E+00
C -3.663862105959E-01 -9.480164558202E-01 -3.449387771889E+00
C 3.432912087589E-01 -2.342538495829E-01 -3.569612911132E+00
C 5.296862811374E-02 4.890991367801E-01 -3.543697678381E+00
C -2.373539525314E-01 1.192428347017E+00 -3.372703046311E+00
C 4.723234668234E-01 1.846939400622E+00 -3.063629555249E+00
C 1.820008861783E-01 2.425836538159E+00 -2.629130710233E+00
C -1.083216944669E-01 2.905419642801E+00 -2.086994945032E+00
C -3.986442751121E-01 3.266054525894E+00 -1.459417361569E+00

C 3.110331442428E-01 3.492976752952E+00 -7.720910598489E-01
C 2.071056359761E-02 3.576896101337E+00 -5.315525942202E-02
C -2.696120170475E-01 3.514376903065E+00 6.679567235710E-01
C 4.400654023073E-01 3.307978701460E+00 1.361722479820E+00
C 1.497428216621E-01 2.966151463147E+00 1.999739157749E+00
C -1.405797589830E-01 2.502889635424E+00 2.555886279600E+00
C -4.309023396282E-01 1.937159211950E+00 3.007395116861E+00
C 2.787750797266E-01 1.292121262732E+00 3.335780844683E+00
H 5.306705562989E-02 -1.062085282325E+00 3.505765661683E+00
H -2.372555250153E-01 -1.746049773675E+00 3.220206237093E+00
H 4.724218943396E-01 -2.358530782139E+00 2.802811190799E+00
H 1.820993136944E-01 -2.874453263267E+00 2.270668725037E+00
H -1.082232669508E-01 -3.272695290062E+00 1.645564814880E+00
H -3.985458475959E-01 -3.536952787157E+00 9.530912878556E-01
H 3.111315717589E-01 -3.656407021572E+00 2.215980915232E-01
H 2.080899111376E-02 -3.626167522914E+00 -5.189673567128E-01
H -2.695135895314E-01 -3.447472299811E+00 -1.238286220389E+00
H 4.401638298234E-01 -3.127637155693E+00 -1.906909500710E+00
H 1.498412491783E-01 -2.679756178939E+00 -2.497463682019E+00
H -1.404813314669E-01 -2.122165669361E+00 -2.985771406748E+00
H -4.308039121120E-01 -1.477693447936E+00 -3.351841299270E+00
H 2.788735072428E-01 -7.727242831310E-01 -3.580686415176E+00
H -1.144907340237E-02 -3.611969538317E-02 -3.662937808532E+00
H -3.017716540475E-01 7.019636369375E-01 -3.595228097629E+00
H 4.079057653073E-01 1.411308495485E+00 -3.380329325989E+00
H 1.175831846621E-01 2.062874218405E+00 -3.027039474570E+00
H -1.727393959830E-01 2.629985628447E+00 -2.549822271401E+00
H -4.630619766282E-01 3.089425117849E+00 -1.968215044849E+00
H 2.466154427267E-01 3.422383179935E+00 -1.306028863105E+00
H -4.370713791850E-02 3.615228472522E+00 -5.903737062541E-01
H -3.340297185637E-01 3.660065886672E+00 1.494514194969E-01
H 3.756477007912E-01 3.555059773382E+00 8.831579865739E-01
H 8.532512014602E-02 3.304509095268E+00 1.580707961914E+00
H -2.049974604991E-01 2.918671426531E+00 2.213543567568E+00
H -4.953200411443E-01 2.413343006662E+00 2.755756439485E+00
H 2.143573782105E-01 1.809212040544E+00 3.185148318982E+00
H -7.596520243462E-02 1.131011720914E+00 3.484139852061E+00
H -3.662877830798E-01 4.065076485405E-01 3.640490290228E+00
H 3.433896362751E-01 -3.346388947265E-01 3.647798628173E+00
H 5.507019097224E-02 -2.089863382477E+00 2.062121672380E+00
H -2.352523896729E-01 -2.462185797156E+00 1.599223514522E+00
H 4.744250296819E-01 -2.733706036005E+00 1.070852958078E+00
H 1.841024490368E-01 -2.893308028544E+00 4.986415557111E-01
H -1.062201316084E-01 -2.934457650444E+00 -9.398429053473E-02
H -3.965427122536E-01 -2.855470231351E+00 -6.827624088834E-01

H 3.131347071013E-01 -2.659579525483E+00 -1.243588153991E+00
H 2.281212645611E-02 -2.354805321355E+00 -1.753501253959E+00
H -2.675104541890E-01 -1.953625110692E+00 -2.191625806562E+00
H 4.421669651658E-01 -1.472463258457E+00 -2.540024941140E+00
H 1.518443845206E-01 -9.310185874126E-01 -2.784435156187E+00
H -1.384781961245E-01 -3.514579060100E-01 -2.914850268782E+00
H -4.288007767697E-01 2.424915033592E-01 -2.925931068893E+00
H 2.808766425851E-01 8.265132820893E-01 -2.817223907262E+00
H -9.445938060018E-03 1.376697509940E+00 -2.593179267857E+00
H -2.997685187052E-01 1.870519579978E+00 -2.262969564541E+00
H 4.099089006497E-01 2.287762358635E+00 -1.840113621364E+00
H 1.195863200045E-01 2.611343877529E+00 -1.341923210325E+00
H -1.707362606407E-01 2.828016671257E+00 -7.887943053859E-01
H -4.610588412858E-01 2.928910130186E+00 -2.033720689049E-01
H 2.486185780690E-01 2.909893664253E+00 3.903762439724E-01
H -4.170400257614E-02 2.771745809807E+00 9.681425075541E-01
H -3.320265832213E-01 2.520122356242E+00 1.506272903125E+00
H 3.776508361335E-01 2.165324797310E+00 1.982736309062E+00
H 8.732825548837E-02 1.721878586761E+00 2.378026257544E+00
H -2.029943251568E-01 1.207938464559E+00 2.675959531637E+00
H -4.933169058020E-01 6.445451996903E-01 2.864338708092E+00
H 2.163605135529E-01 5.476417861560E-02 2.935451521292E+00
H -7.396206709227E-02 -5.372588943661E-01 2.886386604310E+00
H -3.642846477374E-01 -1.107286525087E+00 2.719152680612E+00
H 3.453927716174E-01 -1.631981715371E+00 2.440596326682E+00
H 3.274489649074E-02 -2.511320780200E+00 3.374028376119E+00
H -2.575776841544E-01 -3.139100815145E+00 2.799436660522E+00
H 4.520997352004E-01 -3.638365693890E+00 2.110235679123E+00
H 1.617771545553E-01 -3.988675453637E+00 1.334641401079E+00
H -1.285454260899E-01 -4.175688371663E+00 5.044067472611E-01
H -4.188680067351E-01 -4.191748117130E+00 -3.464783780551E-01
H 2.908094126198E-01 -4.036197202172E+00 -1.183178637864E+00
H 4.868319746114E-04 -3.715403899525E+00 -1.971439425222E+00
H -2.898357486705E-01 -3.242501524689E+00 -2.678989250876E+00
H 4.198416706843E-01 -2.636850756455E+00 -3.276860941832E+00
H 1.295190900391E-01 -1.923247008435E+00 -3.740577560814E+00
H -1.608034906060E-01 -1.130905301918E+00 -4.051154494958E+00
H -4.511260712512E-01 -2.922641994639E-01 -4.195876688087E+00
H 2.585513481036E-01 5.583422336553E-01 -4.168819196612E+00
H -3.177123254152E-02 1.386090070126E+00 -3.971089757411E+00
H -3.220938131867E-01 2.157091216268E+00 -3.610783436960E+00
H 3.875836061682E-01 2.839780794568E+00 -3.102651218350E+00
H 9.726102552300E-02 3.406209413478E+00 -2.467496094314E+00
H -1.930615551222E-01 3.833187418788E+00 -1.731321390259E+00
H -4.833841357673E-01 4.103234280792E+00 -9.242661850655E-01

H 2.262932835875E-01 4.205294249231E+00 -7.937141365840E-02
H -6.402929705764E-02 4.135188977005E+00 7.687728327496E-01
H -3.543518777028E-01 3.895788582197E+00 1.585443429058E+00
H 3.553255416520E-01 3.496894145098E+00 2.337205785099E+00
H 6.500296100687E-02 2.954836450831E+00 2.993282661688E+00
H -2.253196196383E-01 2.291807405089E+00 3.526814194411E+00
H 4.843577997165E-01 1.534951494906E+00 3.915957539633E+00
H 1.940352190714E-01 7.152544901723E-01 4.144781123076E+00
H -9.628736157378E-02 -1.337251174276E-01 4.203916880350E+00
H -3.866099422189E-01 -9.772300030080E-01 4.090943786602E+00
H 3.230674771359E-01 -1.780726977446E+00 3.810486973566E+00
H -2.195580538486E-02 1.475820980898E+00 3.157544210122E+00
H -3.122783860300E-01 8.100018621061E-01 3.389989674014E+00
H 3.973990333248E-01 1.110211719085E-01 3.483648562344E+00
H 1.070764526797E-01 -5.925047381116E-01 3.434686469221E+00
H -1.832461279655E-01 -1.271773434537E+00 3.245107908489E+00
H -4.735687086107E-01 -1.898975577125E+00 2.922674248700E+00
H 2.361087107442E-01 -2.448433436466E+00 2.480585961770E+00
H -5.421386990099E-02 -2.897652143239E+00 1.936942194108E+00
H -3.445364505461E-01 -3.228240630808E+00 1.313999785438E+00
H 3.651409688087E-01 -3.426664567650E+00 6.372620711641E-01
H 7.481838816353E-02 -3.484800454476E+00 -6.556522717843E-02
H -2.155041924816E-01 -3.400268201250E+00 -7.657082774167E-01
H 4.941732268732E-01 -3.176528568349E+00 -1.434503140811E+00
H 2.038506462280E-01 -2.822741482634E+00 -2.044569277073E+00
H -8.647193441712E-02 -2.353391028962E+00 -2.570930506905E+00
H -3.767945150623E-01 -1.787692470053E+00 -2.992037539713E+00
H 3.328829042926E-01 -1.148805571374E+00 -3.290650204095E+00
H 4.256032364740E-02 -4.628864376250E-01 -3.454543262487E+00
H -2.477622569978E-01 2.419833212675E-01 -3.477006913821E+00
H 4.619151623571E-01 9.369462545555E-01 -3.357121493573E+00
H 1.715925817119E-01 1.593550498096E+00 -3.099795124932E+00
H -1.187299989332E-01 2.184914597009E+00 -2.715562779666E+00
H -4.090525795784E-01 2.686828035605E+00 -2.220154975136E+00
H 3.006248397764E-01 3.078742418734E+00 -1.633853765066E+00
H 1.030225913127E-02 3.344612725503E+00 -9.806623898853E-01
H -2.800203215139E-01 3.473554194315E+00 -2.873225812394E-01
H 4.296570978409E-01 3.460287946286E+00 4.177802476415E-01
H 1.393345171958E-01 3.305357103170E+00 1.105779104097E+00
H -1.509880634494E-01 3.015104551887E+00 1.748507234107E+00
H -4.413106440945E-01 2.601413265990E+00 2.319651272512E+00
H 2.683667752603E-01 2.081219815330E+00 2.795828515272E+00
H 3.059316054186E-03 8.996224581608E-01 4.276017559208E+00
H -2.872632645910E-01 2.045112704998E-02 4.369579898032E+00
H 4.224141547639E-01 -8.595574756052E-01 4.284251122427E+00

H 1.320915741187E-01 -1.704375694215E+00 4.023524602491E+00
H -1.582310065265E-01 -2.479416571649E+00 3.598074512585E+00
H -4.485535871716E-01 -3.152949843320E+00 3.025318829379E+00
H 2.611238321832E-01 -3.697400977949E+00 2.328706237837E+00
H -2.919874846194E-02 -4.090480082115E+00 1.536756139308E+00
H -3.195213291071E-01 -4.316094451109E+00 6.818910638734E-01
H 3.901560902477E-01 -4.365007406154E+00 -2.008907118346E-01
H 9.983350960257E-02 -4.235216445125E+00 -1.075447998196E+00
H -1.904890710426E-01 -3.932035225216E+00 -1.905976317152E+00
H -4.808116516877E-01 -3.467876021191E+00 -2.658473741741E+00
H 2.288657676671E-01 -2.861741565402E+00 -3.302132938986E+00
H -6.145681297807E-02 -2.138447073684E+00 -3.810602425724E+00
H -3.517793936232E-01 -1.327604307512E+00 -4.163065401427E+00
H 3.578980257316E-01 -4.624092650047E-01 -4.345091990455E+00
H 6.757544508644E-02 4.217168671431E-01 -4.349230002868E+00
H -2.227471355587E-01 1.288577861200E+00 -4.175310027951E+00
H 4.869302837961E-01 2.102684326219E+00 -3.830452369911E+00
H 1.966077031510E-01 2.830706647867E+00 -3.328775541788E+00
H -9.371487749420E-02 3.442839506757E+00 -2.690818251870E+00
H -3.840374581394E-01 3.914022111725E+00 -1.942698546562E+00
H 3.256399612155E-01 4.224964191560E+00 -1.115044534501E+00
H 3.531738057032E-02 4.362935740980E+00 -2.417404681847E-01
H -2.550052000748E-01 4.322288188542E+00 6.414604813019E-01
H 4.546722192800E-01 4.104685649818E+00 1.498399963316E+00
H 1.643496386348E-01 3.719036798309E+00 2.293994774777E+00
H -1.259729420103E-01 3.181130143310E+00 2.995673170626E+00
H -4.162955226555E-01 2.512987646477E+00 3.574708354892E+00
H 2.933818966994E-01 1.741963140133E+00 4.007394559099E+00
H -2.612996741720E-02 -7.215073114984E-02 3.987519762827E+00
H -3.164525480624E-01 -8.733556285259E-01 3.891371163621E+00
H 3.932248712925E-01 -1.638805243855E+00 3.635909371760E+00
H 1.029022906473E-01 -2.337161979950E+00 3.231593023018E+00
H -1.874202899978E-01 -2.939835029980E+00 2.694974876218E+00
H -4.777428706430E-01 -3.422150888467E+00 2.048024141339E+00
H 2.319345487118E-01 -3.764363487495E+00 1.317227057481E+00
H -5.838803193333E-02 -3.952462603050E+00 5.325025431217E-01
H -3.487106125785E-01 -3.978747435242E+00 -2.740226879189E-01
H 3.609668067764E-01 -3.842141879953E+00 -1.069329397920E+00
H 7.064422613119E-02 -3.548238584665E+00 -1.820857636729E+00
H -2.196783545140E-01 -3.109069984821E+00 -2.497839749949E+00
H 4.899990648409E-01 -2.542615694498E+00 -3.072560010322E+00
H 1.996764841957E-01 -1.872066418898E+00 -3.521489302863E+00
H -9.064609644946E-02 -1.124874524150E+00 -3.826248409586E+00
H -3.809686770946E-01 -3.316301342157E-01 -3.974360456856E+00
H 3.287087422602E-01 4.751912323782E-01 -3.959761720055E+00

H 3.838616161506E-02 1.262558214086E+00 -3.783049873182E+00
H -2.519364190301E-01 1.998235914165E+00 -3.451459520012E+00
H 4.577410003247E-01 2.652105601135E+00 -2.978566008564E+00
H 1.674184196796E-01 3.197397773185E+00 -2.383729654758E+00
H -1.229041609656E-01 3.611788104723E+00 -1.691303128810E+00
H -4.132267416107E-01 3.878311406887E+00 -9.296344540487E-01
H 2.964506777441E-01 3.986056184370E+00 -1.299064355113E-01
H 6.128097098930E-03 3.930611353323E+00 6.751399677592E-01
H -2.841944835462E-01 3.714246831645E+00 1.452546061424E+00
H 4.254829358086E-01 3.345820608273E+00 2.170484748667E+00
H 1.351603551634E-01 2.840416096081E+00 2.799563535279E+00
H -1.551622254817E-01 2.218724615181E+00 3.314027861822E+00
H -4.454848061269E-01 1.506198287847E+00 3.692815498320E+00
H 2.641926132280E-01 7.320080256368E-01 3.920418834429E+00

PbE0/POB-TZVP optimized geometry, *all*-[38.4]-$(PbMe_2)_\infty$

Energy (a.u): -1.3630334717729E+03
Unit cell length (Å): 7.05906623

Pb	2.232580464669E-01	1.836526763908E-01	2.190479117488E+00
Pb	1.635071292467E+00	-2.026517640428E+00	8.515593477437E-01
Pb	3.046884538467E+00	-1.436109456977E+00	-1.664186497145E+00
Pb	-2.600368445533E+00	1.138953184451E+00	-1.880083166598E+00
Pb	-1.188555199533E+00	2.140021236563E+00	5.022311985107E-01
C	2.125804749306E+00	1.139838152272E+00	2.955436964114E+00
C	-3.521448234694E+00	-2.458558223331E+00	1.997330749955E+00
C	-2.109634988694E+00	-2.659310697611E+00	-1.721018673866E+00
C	-6.978217426935E-01	8.150138255613E-01	-3.060978785678E+00
C	7.139915033065E-01	3.163016943109E+00	-1.707702545250E-01
C	-6.304854479885E-01	-8.583169065262E-01	3.995463128671E+00
C	7.813277980115E-01	-4.065145754816E+00	4.183581201598E-01
C	2.193141044012E+00	-1.654081339172E+00	-3.736903590943E+00
C	-3.454111939988E+00	3.042867267050E+00	-2.727891552044E+00
C	-2.042298693988E+00	3.534676733464E+00	2.050973894156E+00
H	1.895618468868E+00	2.015523283275E+00	3.561763280752E+00
H	3.307431714868E+00	-2.764607230570E+00	3.017521935996E+00
H	-2.339821269132E+00	-3.724144517311E+00	-1.696832162508E+00
H	-9.280080231317E-01	4.629593398550E-01	-4.066221885630E+00
H	4.838052228683E-01	4.010269124750E+00	-8.162311686103E-01
H	2.715496448891E+00	1.445139874404E+00	2.093167465884E+00
H	-2.931756535109E+00	-1.544147777686E+00	2.021234013541E+00
H	-1.519943289109E+00	-2.399475684667E+00	-8.439761462984E-01
H	-1.081300431095E-01	6.119024938331E-02	-2.542839957647E+00
H	1.303683202891E+00	2.437293338566E+00	-7.275853754790E-01
H	2.695884734474E+00	4.287829730375E-01	3.551244755953E+00
H	-2.951368249526E+00	-3.244933240541E+00	1.505191821358E+00
H	-1.539555003526E+00	-2.434262006916E+00	-2.620985050765E+00
H	-1.277417575263E-01	1.740476582744E+00	-3.125049666736E+00
H	1.284071488474E+00	3.509935691675E+00	6.895981401907E-01
H	-1.070547474819E+00	-1.174119216336E-01	4.661455841311E+00
H	3.412657711806E-01	-4.469590232428E+00	1.328803700333E+00
H	1.753079017181E+00	-2.644946757791E+00	-3.840209990129E+00
H	3.164892263181E+00	2.834923237679E+00	-3.702183998169E+00
H	-2.482360720819E+00	4.397025674174E+00	1.552134446654E+00
H	1.688702833039E-01	-1.376526117977E+00	4.521764332995E+00
H	1.580683529304E+00	-4.725823397702E+00	8.814788910146E-02
H	2.992496775304E+00	-1.544193366632E+00	-4.467285941494E+00
H	-2.654756208696E+00	3.771459411921E+00	-2.849082438409E+00
H	-1.242942962696E+00	3.875083470390E+00	2.706456157806E+00

H -1.395253702573E+00 -1.572326103756E+00 3.701056508472E+00
H 1.655954342713E-02 -4.005789396319E+00 -3.516816284583E-01
H 1.428372789427E+00 -9.033878949430E-01 -3.918407708078E+00
H 2.840186035427E+00 3.447464972219E+00 -2.070027516914E+00
H -2.807066948573E+00 3.034038422799E+00 2.639060344978E+00