Supporting information

To

DO DIRADICALS BEHAVE LIKE RADICALS?

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S1. The derivation of Eqs. 6, 9 and 10

The derivation of the energy expressions for the different states of a diradical starts by considering a single set of orbitals that is an acceptable approximation for the actual sets of orbitals of the different states. We will not consider the exact form of this hypothetical set of (frozen) orbitals since this plays no role in the following derivation.

With this set of frozen orbitals, the different states of a diradical can now be formed by filling up the Molecular Spin Orbitals (MSOs) accordingly. From this approximate wave function, an estimate of the energy of the corresponding state can then be determined by calculating the expectation value of the Hamiltonian operator in a Hartree-Fock framework.

Let us start by considering the simplest case of all, the triplet state of a diradical. The approximate wave function for this state can be obtained by filling all the lower lying MSOs up to $\psi_x^{\alpha/\beta}$ and $\psi_y^{\alpha/\beta}$ and then placing the two remaining electrons for example in ψ_x^{α} and ψ_y^{α} or ψ_x^{β} and ψ_y^{β}. Focusing on the α-MSOs here and not explicitly treating the lower lying filled orbitals, the approximate wave function Ψ_T can then be written as $|\ldots \psi_x^{\alpha}\ \psi_y^{\alpha}\rangle$ (corresponding to configuration (c) in Fig. 4 of the main text. The energy of this wave function can then be determined in a Hartree-Fock framework as follows,

$$\mathrm{E}_T = \langle \Psi_T | H | \Psi_T \rangle = \sum_i h_i + \frac{1}{2} \sum_i \sum_j (J_{ij} - K_{ij}) \,, \qquad \text{(S1.1)}$$

with h_i the one-electron integrals corresponding to electrons occupying the respective approximate orbitals and J_{ij}, K_{ij} corresponding to the Coulomb and exchange integrals. We stress here one more time that an approximate wave function is being used so that the terms in Eq. S1.1 do not correspond exactly to the ones that would be obtained for the wave function obtained with a full Hartree-Fock approach.

Eq. S1.1 can then further be written as

$$\mathrm{E}_T = E' + \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(J_{xx} - K_{xx} + J_{yy} - K_{yy} + J_{xy} - K_{xy} + J_{yx} - K_{yx}\right). \quad \text{(S1.2)}$$

Here, E' corresponds to the one electron integrals of the electrons in the lower lying MSOs together with the interactions between them, $\tilde{h}_x$ and $\tilde{h}_y$ correspond to the one electron integrals of orbitals x and y respectively, combined with all the repulsion and exchange interactions of the electron in these orbitals with all electrons in lower lying MSOs (corresponding to a fixed value). Since E' will be the same for every single state and we are interested in the relative ordering of the respective states, we will move the origin of the energy axis to this value. As such, we can write,

$$\mathrm{E}_T = \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(J_{xx} - K_{xx} + J_{yy} - K_{yy} + J_{xy} - K_{xy} + J_{yx} - K_{yx}\right). \quad \text{(S1.3)}$$

Given that by definition $J_{xx} = K_{xx}$ and $J_{yy} = K_{yy}$, Eq. S1.2 can be simplified to,

$$\mathrm{E}_T = \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(2J_{xy} - 2K_{xy}\right) = \tilde{h}_x + \tilde{h}_y + J_{xy} - K_{xy}\,, \quad \text{(S1.4)}$$

Which corresponds exactly to Eq. 6 of the main text.

The approximate form of the open-shell singlet wave function can be constructed analogously to the construction of the wave function of the triplet state by filling up the orbitals according to the configurations (e) and (f) in the main text, and then, in order to obtain an S^2 eigenfunction, combining them linearly as in Eq. S1.5,

$$\Psi_{S_{OS}} = \frac{1}{\sqrt{2}}\left(\left|\ldots \psi_x^\alpha\, \psi_y^\beta\right\rangle - \left|\ldots \psi_x^\beta\, \psi_y^\alpha\right\rangle\right). \quad \text{(S1.5)}$$

The approximate energy can then be obtained as follows,

$$\begin{aligned} \mathrm{E}_{S_{OS}} &= \langle \Psi_{S_{OS}} | H | \Psi_{S_{OS}} \rangle \\ &= \frac{1}{2}\Big[\Big\langle \dots \psi_x^\alpha \psi_y^\beta \Big| H \Big| \dots \psi_x^\alpha \psi_y^\beta \Big\rangle + \Big\langle \dots \psi_x^\beta \psi_y^\alpha \Big| H \Big| \dots \psi_x^\beta \psi_y^\alpha \Big\rangle \\ &- \Big\langle \dots \psi_x^\alpha \psi_y^\beta \Big| H \Big| \dots \psi_x^\beta \psi_y^\alpha \Big\rangle - \Big\langle \dots \psi_x^\beta \psi_y^\alpha \Big| H \Big| \dots \psi_x^\alpha \psi_y^\beta \Big\rangle \Big], \end{aligned} \tag{S1.6}$$

The first two terms in Eq. S1.6 correspond to the energy of a wave function described by a single Slater Determinant (SD). As such, the contributions of these terms can be determined as follows,

$$\Big\langle \dots \psi_x^\alpha \psi_y^\beta \Big| H \Big| \dots \psi_x^\alpha \psi_y^\beta \Big\rangle = \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(J_{xy} - K_{xy} + J_{yx} - K_{yx}\right). \tag{S1.7}$$

Since the two electrons have different spin, $K_{xy} = 0$. As such, Eq. S1.7 can be simplified to

$$\Big\langle \dots \psi_x^\alpha \psi_y^\beta \Big| H \Big| \dots \psi_x^\alpha \psi_y^\beta \Big\rangle = \tilde{h}_x + \tilde{h}_y + J_{xy}\,, \tag{S1.8}$$

The final two terms in Eq. S1.6 correspond to the energy contribution of a double excitation. These terms can then be determined as follows,[1]

$$\begin{aligned} &\Big\langle \dots \psi_x^\alpha \psi_y^\beta \Big| H \Big| \dots \psi_x^\beta \psi_y^\alpha \Big\rangle \\ &= \langle \psi_x \alpha(1) \psi_y \beta(2) | \psi_x \beta(1) \psi_y \alpha(2) \rangle \\ &- \langle \psi_x \alpha(1) \psi_y \beta(2) | \psi_x \beta(2) \psi_y \alpha(1) \rangle . \end{aligned} \tag{S1.9}$$

The first term in this expression is equal to zero because of the orthogonality of the spin functions, so that,

$$\Big\langle \dots \psi_x^\alpha \psi_y^\beta \Big| H \Big| \dots \psi_x^\beta \psi_y^\alpha \Big\rangle = -\langle \psi_x \alpha(1) \psi_y \beta(2) | \psi_x \beta(2) \psi_y \alpha(1) \rangle = -K_{xy}\,. \tag{S1.10}$$

Filling Eqs. S1.8 and S1.10 into Eq. S1.6, we obtain,

$$\mathrm{E}_{S_{OS}} = \tilde{h}_x + \tilde{h}_y + J_{xy} + K_{xy}\,, \tag{S1.11}$$

which corresponds to Eq. 9 in the main text.

The lowest-lying closed-shell singlet wave function can be constructed completely analogously to the open-shell singlet wave function by combining configurations (a) and (b),

$$\Psi_{S_{CS-}} = \frac{1}{\sqrt{2}}\left(\left|\ldots \psi_x^\alpha \, \psi_x^\beta\right\rangle - \left|\ldots \psi_y^\alpha \, \psi_y^\beta\right\rangle\right). \tag{S1.12}$$

The energy of this wave function can be expressed as follows,

$$\begin{aligned} \mathrm{E}_{S_{CS-}} &= \left\langle \Psi_{S_{CS-}} \middle| H \middle| \Psi_{S_{CS-}} \right\rangle \\ &= \frac{1}{2}\left[\left\langle \ldots \psi_x^\alpha \psi_x^\beta \middle| H \middle| \ldots \psi_x^\alpha \psi_x^\beta \right\rangle + \left\langle \ldots \psi_y^\alpha \psi_y^\beta \middle| H \middle| \ldots \psi_y^\alpha \psi_y^\beta \right\rangle \right. \\ &\left. - \left\langle \ldots \psi_x^\alpha \psi_x^\beta \middle| H \middle| \ldots \psi_y^\alpha \psi_y^\beta \right\rangle - \left\langle \ldots \psi_y^\alpha \psi_y^\beta \middle| H \middle| \ldots \psi_x^\alpha \psi_x^\beta \right\rangle\right]. \end{aligned} \tag{S1.13}$$

Again, the first two terms in Eq. S1.6 correspond to the energy of a wave function described by a single Slater Determinant (SD). As such, the contributions of these terms can be determined as,

$$\left\langle \ldots \psi_x^\alpha \psi_x^\beta \middle| H \middle| \ldots \psi_x^\alpha \psi_x^\beta \right\rangle = \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(J_{xx} + J_{yy}\right). \tag{S1.14}$$

The two final terms correspond once more correspond to the energy contribution of a double excitation. These terms can then be determined as follows,

$$\begin{aligned} &\left\langle \ldots \psi_x^\alpha \psi_x^\beta \middle| H \middle| \ldots \psi_y^\alpha \psi_y^\beta \right\rangle \\ &= \left\langle \psi_x \alpha(1) \psi_x \beta(2) \middle| \psi_y \alpha(1) \psi_y \beta(2) \right\rangle \\ &- \left\langle \psi_x \alpha(1) \psi_x \beta(2) \middle| \psi_y \alpha(2) \psi_y \beta(1) \right\rangle. \end{aligned} \tag{S1.15}$$

The second term in this expression is equal to zero (orthogonality of the spin function), so that,

$$\left\langle \ldots \psi_x^\alpha \psi_y^\beta \middle| H \middle| \ldots \psi_x^\beta \psi_y^\alpha \right\rangle = \left\langle \psi_x \alpha(1) \psi_x \beta(2) \middle| \psi_y \alpha(1) \psi_y \beta(2) \right\rangle = K_{xy}. \tag{S1.16}$$

Filling Eqs. S1.15 and S1.16 into Eq. S1.13, we finally obtain,

$$\mathrm{E}_{S_{CS-}} = \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(J_{xx} + J_{yy}\right) - K_{xy}. \tag{S1.17}$$

In complete analogy, the energy for the second closed-shell singlet configuration can be obtained as,

$$\mathrm{E}_{S_{CS+}} = \tilde{h}_x + \tilde{h}_y + \frac{1}{2}\left(J_{xx} + J_{yy}\right) + K_{xy}. \tag{S1.18}$$

These expressions correspond exactly to Eq. 10 in the main text.

Applying this framework to the (symmetric) diradical O_2, the ordering and the approximate spacing of the different spectroscopic terms can be obtained (see Fig. 5). In this case $E_{S_{CS-}}$ and $E_{S_{OS}}$ are identical due to symmetry, corresponding to the $^1\Delta_g^+$ and $^1\Delta_g^-$ states respectively, E_T corresponds to the $^3\Sigma_g^+$ and $E_{S_{CS+}}$ to the $^1\Sigma_g^+$ terms, lying $2K_{xy}$ below and above the $^1\Delta_g^{+/-}$ states (see also Section 10.1.7).

S2. Active Spaces for the CASPT2 Calculations

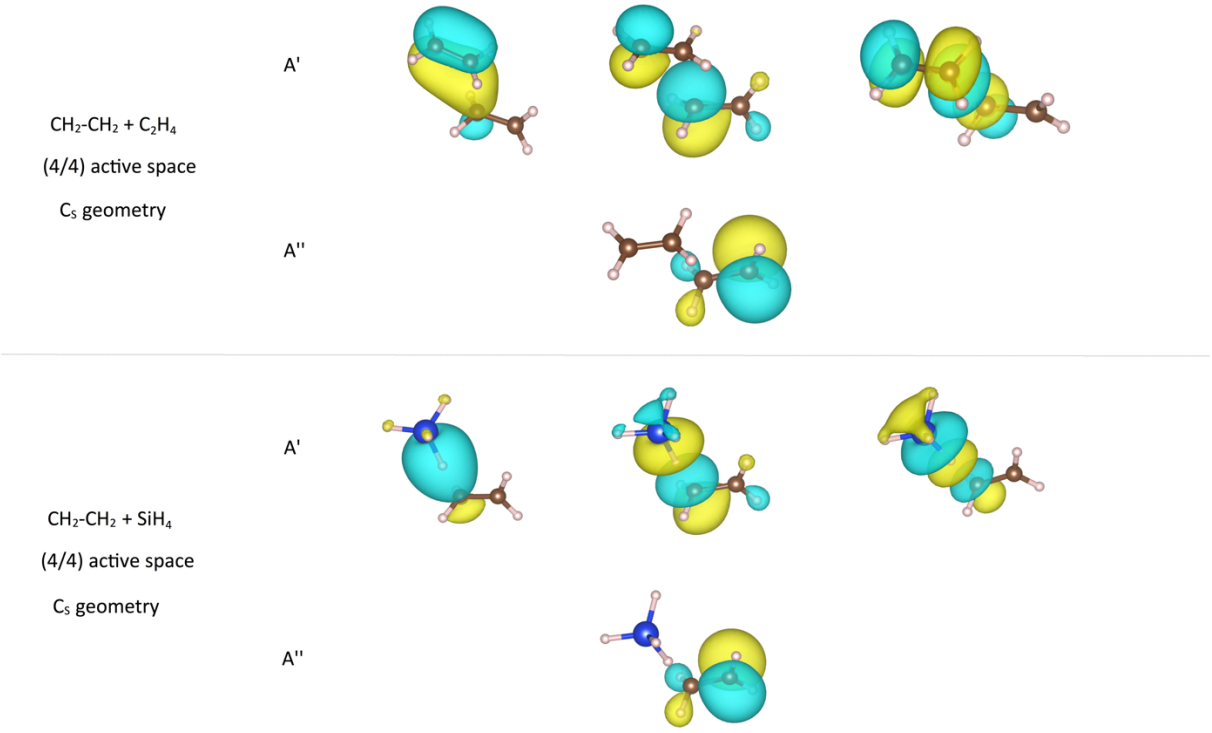

Figure S2.1. The active spaces chosen in the CASPT2 calculations for •CH_2-CH_2•.

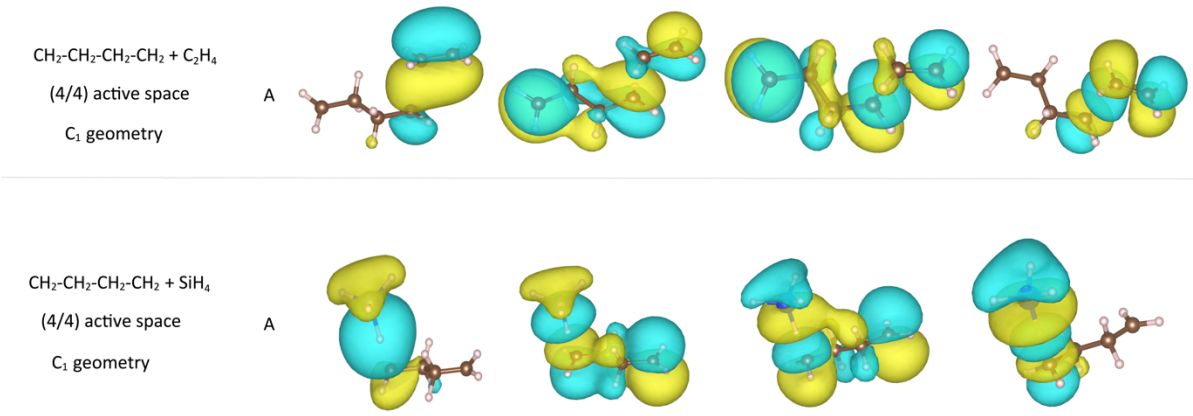

Figure S2.2. The active spaces chosen in the CASPT2 calculations for •CH_2-CH_2-CH_2-CH_2•.

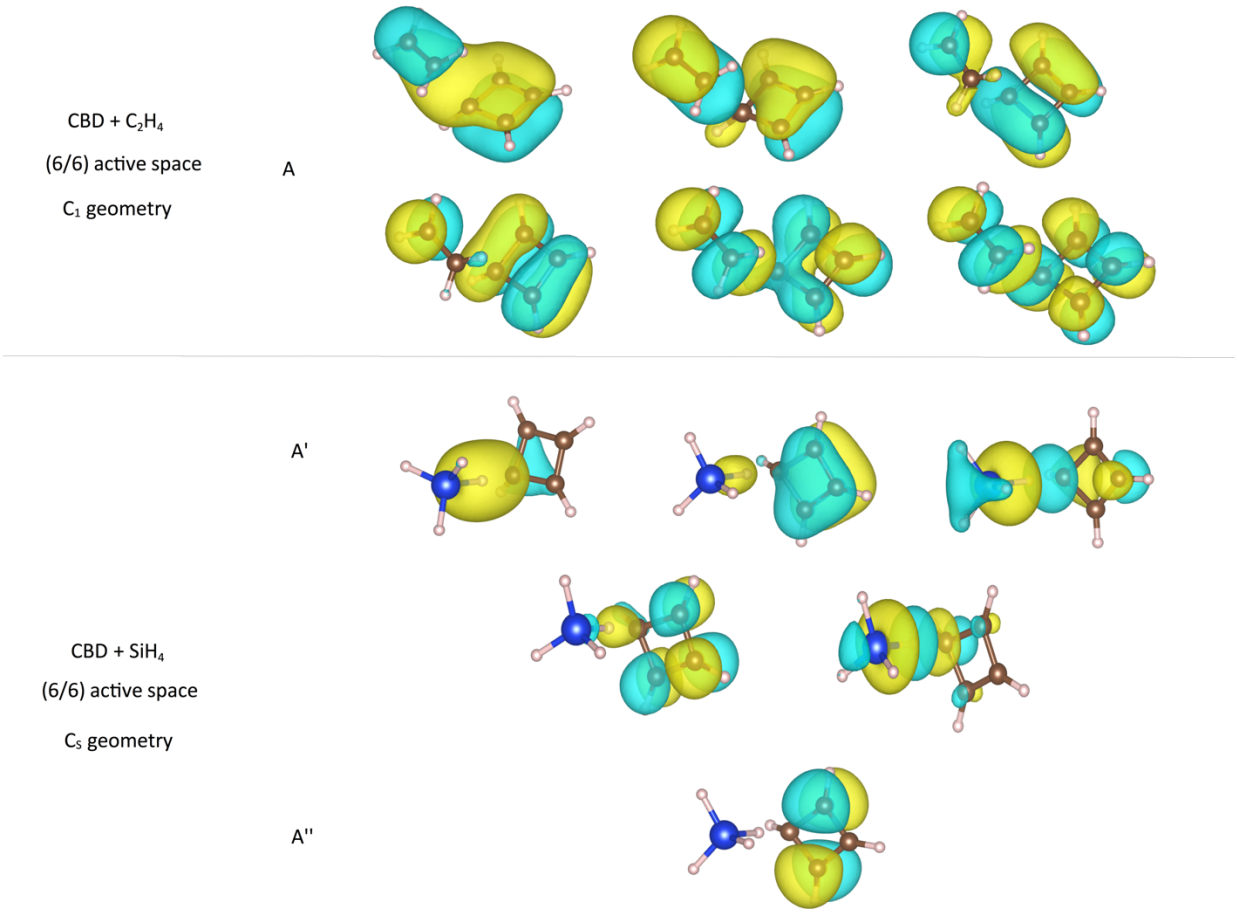

Figure S2.3. The active spaces chosen in the CASPT2 calculations for CBD.

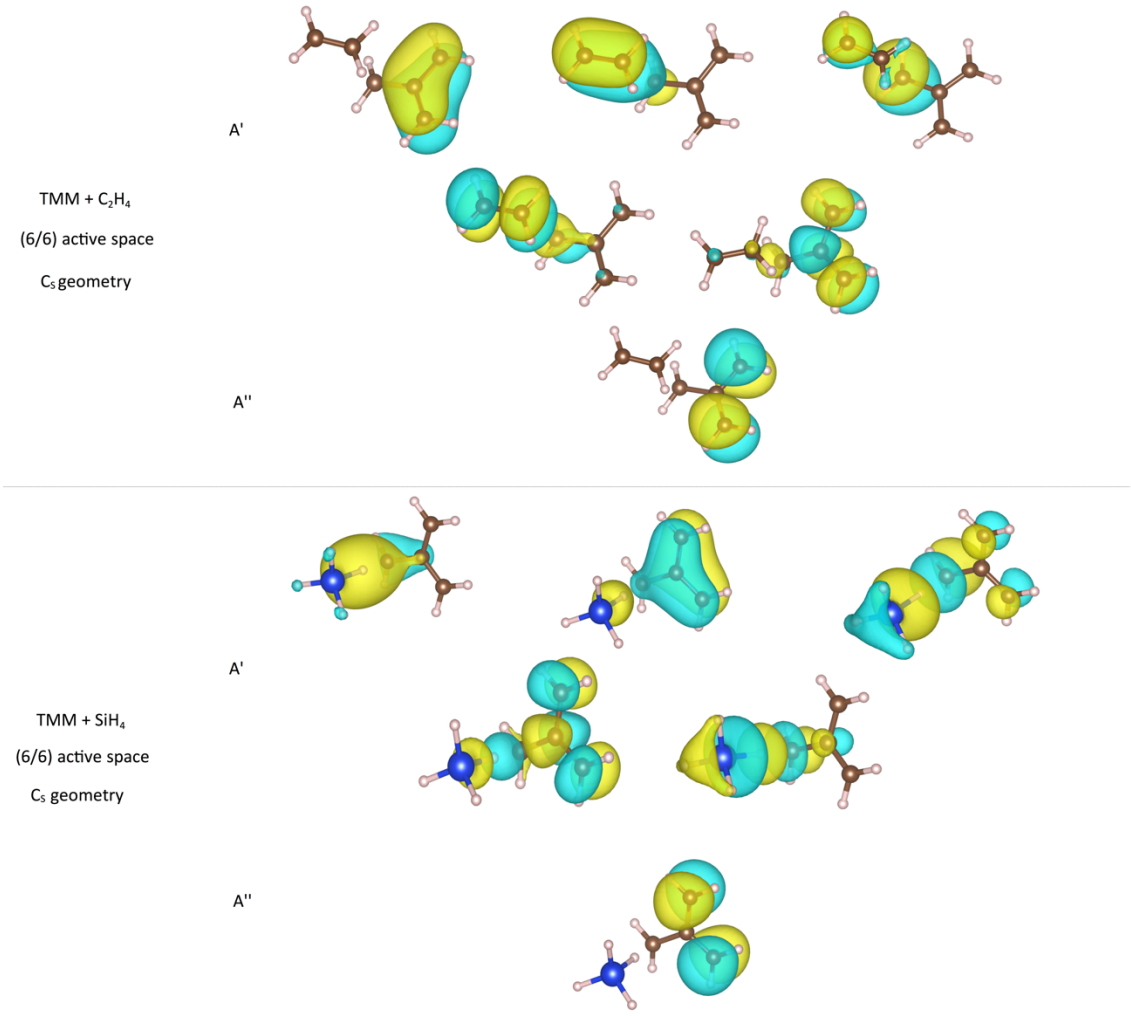

Figure S2.4. The active spaces chosen in the CASPT2 calculations for TMM.

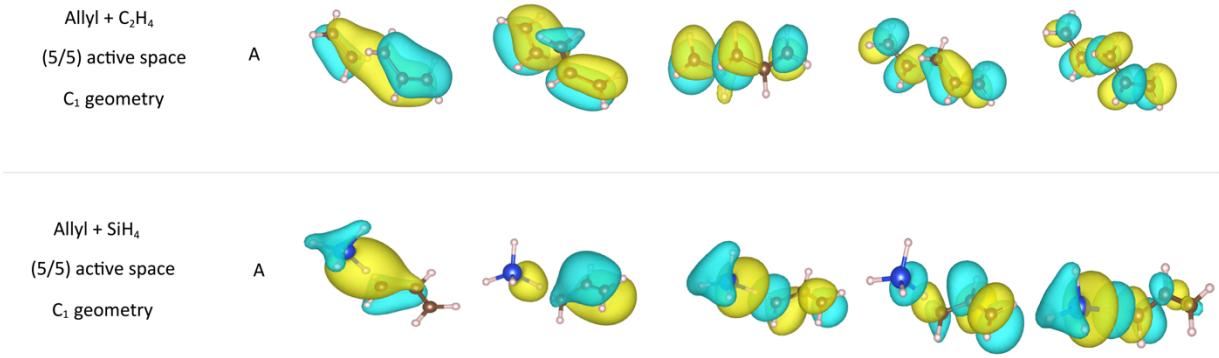

Figure S2.5. The active spaces chosen in the CASPT2 calculations for allyl.

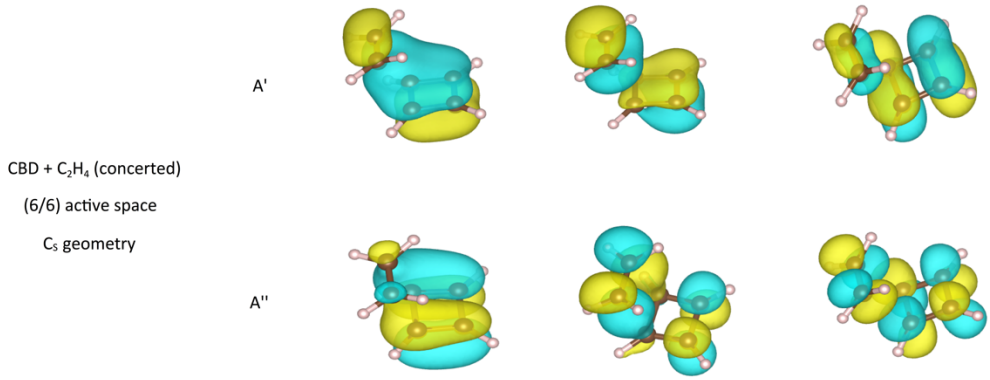

Figure S2.6. The active space chosen in the CASPT2 calculations of the concerted addition reaction to ethylene for CBD.

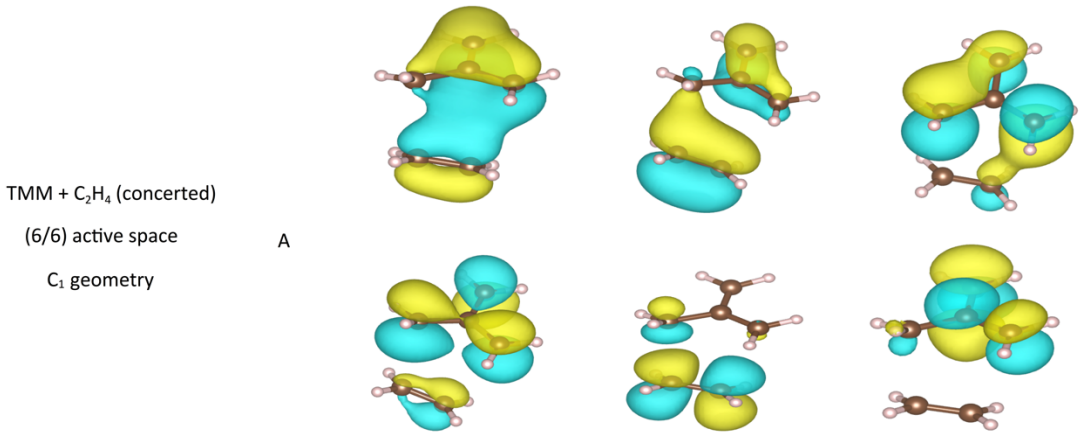

Figure S2.7. The active space chosen in the CASPT2 calculations of the concerted addition reaction to ethylene for TMM.

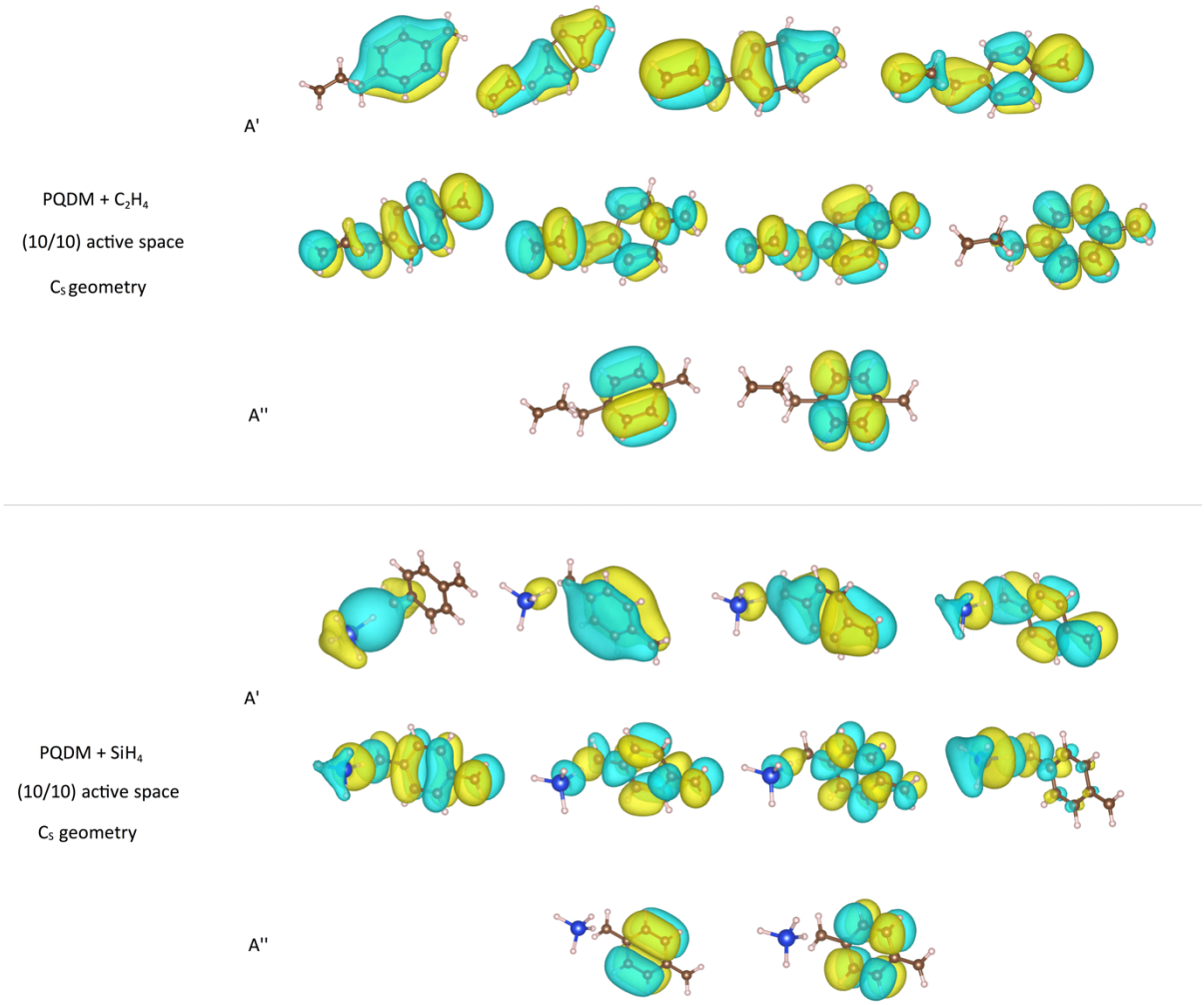

Figure S2.8. The active spaces chosen in the CASPT2 calculations for PQDM.

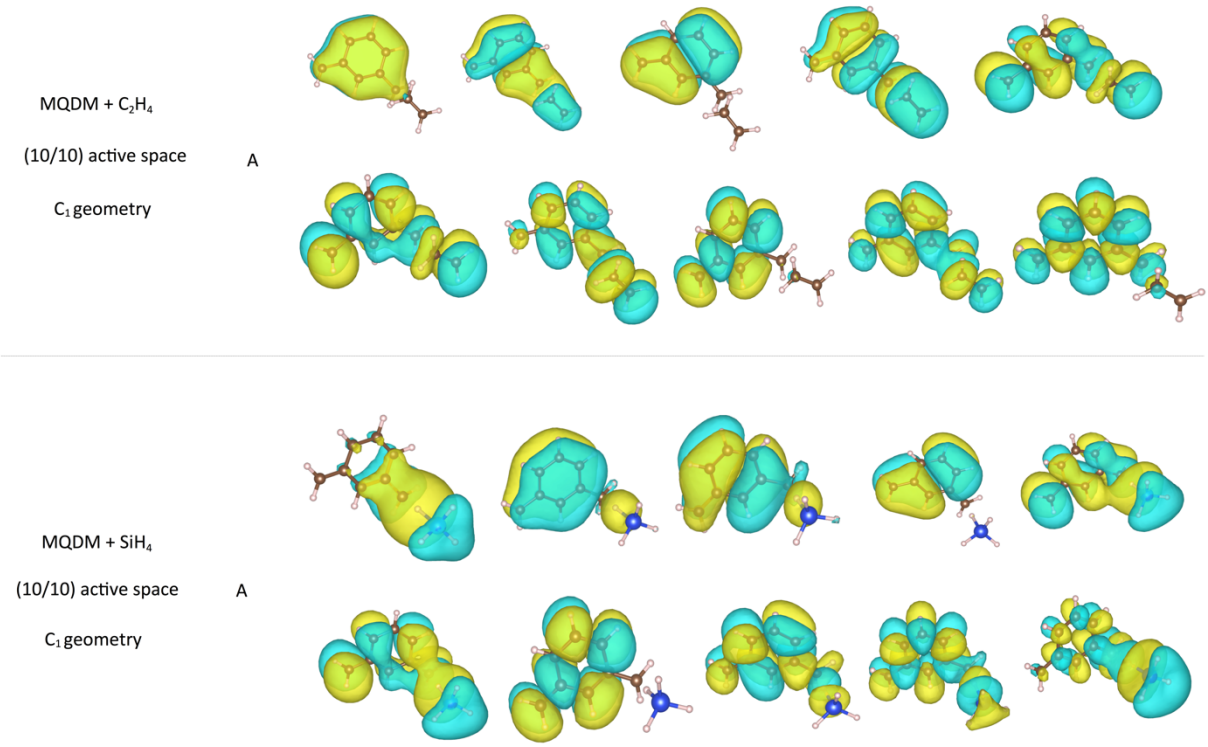

Figure S2.9. The active spaces chosen in the CASPT2 calculations for MQDM.

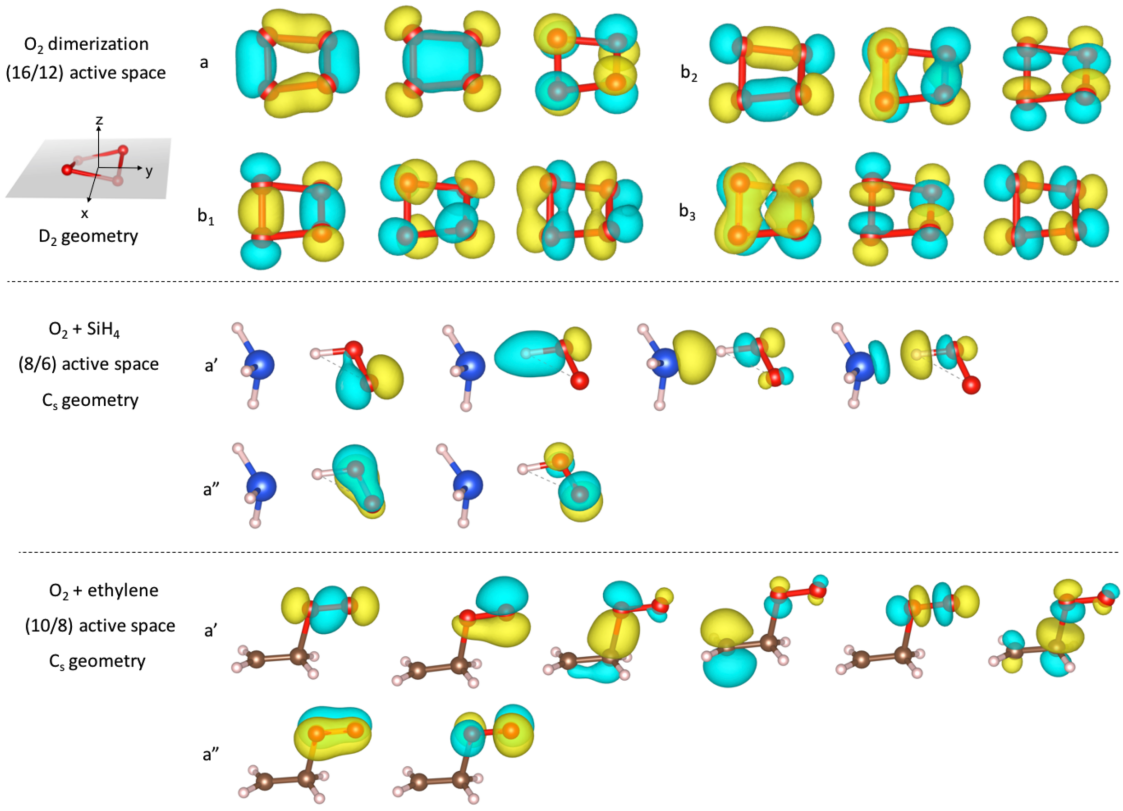

Figure S2.10. The active spaces chosen in the CASPT2 calculations for O_2.

S3. GVB transformation of the frontier orbitals associated to $C_5H_5^+$ and $C_3H_3^-$

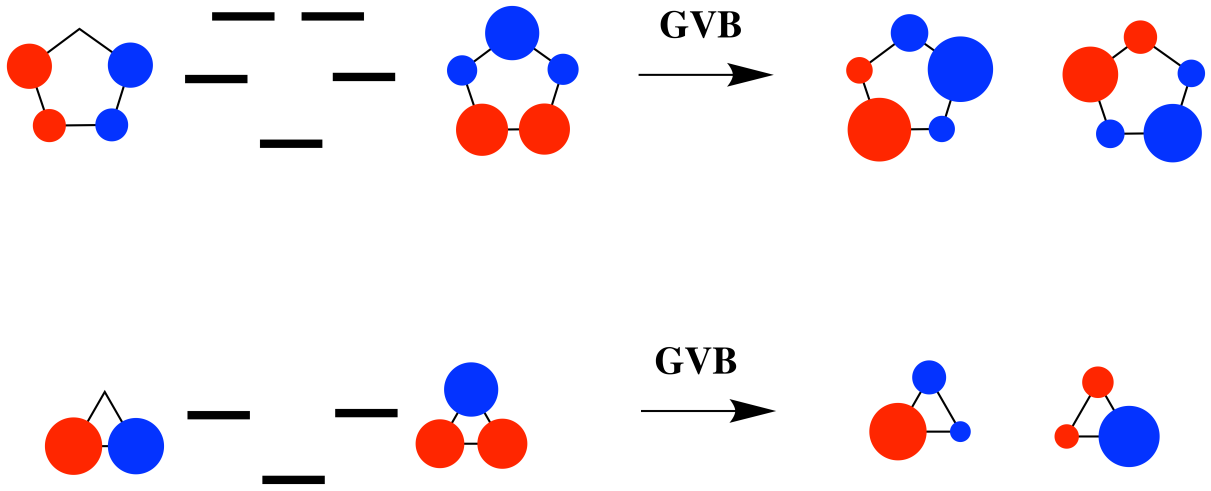

Figure S3.1. The GVB orbital transformation for $C_5H_5^+$ (D_{5h}) and $C_3H_3^-$ (D_{3h}).

S4. The singlet wave function(s) for O_2

Given the axis convention of Figure S3.1 (molecule oriented along z axis), the open-shell

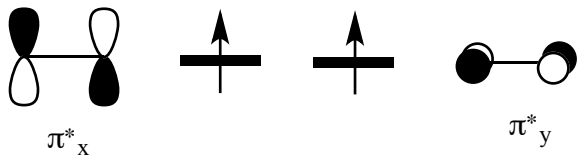

Figure S4.1. The π_x^* and π_y^* molecular orbitals of O_2. The molecule lies along the z axis.

singlet wave function for O_2 can be written as[2]

$$\Psi_{S_{OS}} = \frac{\left(\left|\pi^{*\alpha}_x(1)\pi^{*\beta}_y(2)\right\rangle - \left|\pi^{*\beta}_x(1)\pi^{*\alpha}_y(2)\right\rangle\right)}{\sqrt{2}} = \frac{\left[\pi^*_x(1)\pi^*_y(2) + \pi^*_y(1)\pi^*_x(2)\right]\left[\alpha(1)\beta(2) - \beta(1)\alpha(2)\right]}{2}. \quad \text{(S4.1)}$$

All the other occupied orbitals have been omitted. For the lower closed-shell singlet $\Psi_{S_{CS-}}$,

$$\Psi_{S_{CS-}} = \frac{\left|\pi_x^{*2}\right\rangle - \left|\pi_y^{*2}\right\rangle}{\sqrt{2}}$$

Performing the GVB transformation (see Figure S4.2),

$$\pi_{x'}^{*} = \left(\frac{\pi_x^{*} + \pi_y^{*}}{\sqrt{2}}\right), \tag{S4.2}$$

and

$$\pi_{y'}^{*} = \left(\frac{\pi_x^{*} - \pi_y^{*}}{\sqrt{2}}\right). \tag{S4.3}$$

we have

$$\begin{aligned}\Psi_{S_{CS-}} &= \frac{\left|\pi_x^{*2}\right\rangle - \left|\pi_y^{*2}\right\rangle}{\sqrt{2}} = \frac{\left|\pi_{x'}^{*\alpha}(1)\pi_{y'}^{*\beta}(2)\right\rangle - \left|\pi_{x'}^{*\beta}(1)\pi_{y'}^{*\alpha}(2)\right\rangle}{\sqrt{2}} \\ &= \frac{\left[\pi_{x'}^{*}(1)\pi_{y'}^{*}(2) + \pi_{x'}^{*}(2)\pi_{y'}^{*}(1)\right][\alpha(1)\beta(2) - \beta(1)\alpha(2)]}{2}.\end{aligned} \tag{S4.4}$$

Since the spatial orientation of the *x* and *y* coordinate axes in O_2 is purely arbitrary, this means that the energies of the "open-shell" singlet wave function and the "closed-shell" singlet wave function must be the same; i.e., these two states are degenerate (Figure S4.2).[2] The lowest singlet state of O_2 is indeed doubly degenerate $^1\Delta_g$.

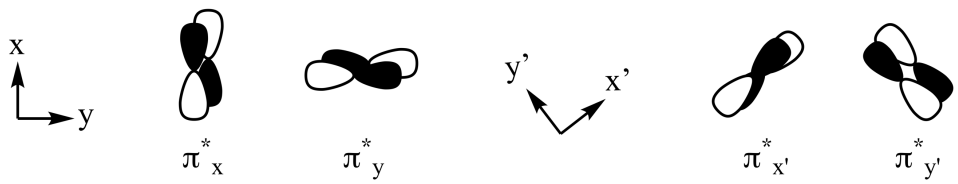

Figure S4.2. Conventional MOs (left) and GVB orbitals (right) for O_2.

S5. Orbital Correlation Diagram Analysis for the Dimerization Reaction of O_2

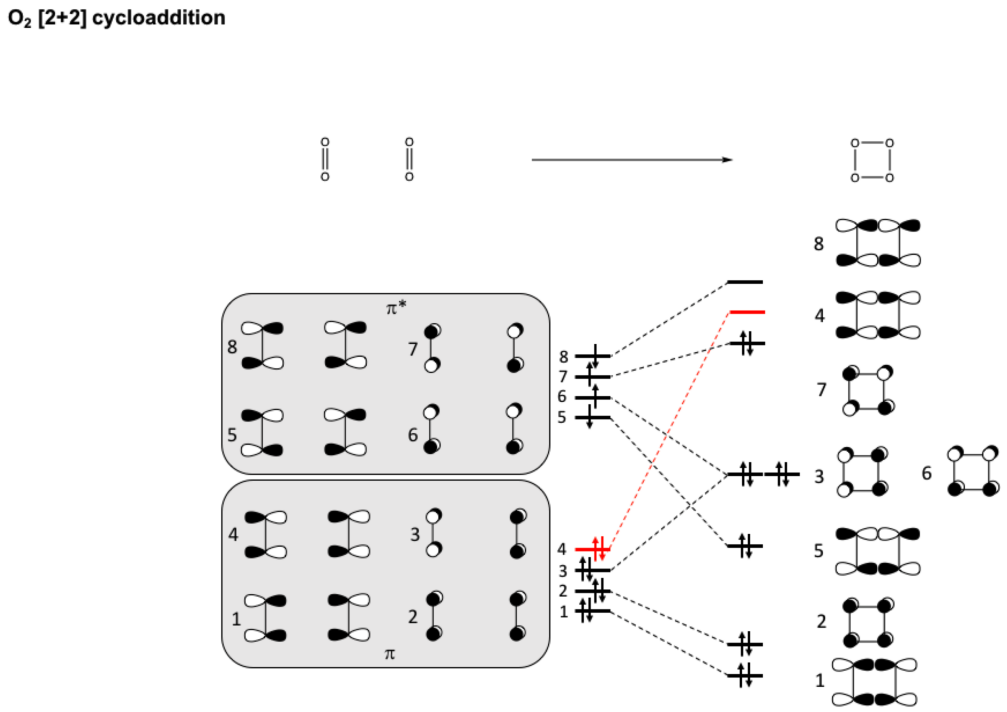

Figure S5.1. Orbital correlation diagram for the O_2 [2+2] cycloaddition reaction.

S6. The Preparation Perspective on the Closed-shell Reactivity of Diradicaloids

S6.1. Closed-shell Reactivity of Closed-shell Molecules

From an MO point of view, the nucleophilic addition of methyl anion to ethylene (Figure S6.1) is similar to the radical reaction above, except for an additional electron. This changes the radical to an anion, and pushes up the ψ_1 level so that ψ_1 is closer in energy to the π^* level (a typical feature of anions); the interaction between these two orbitals polarizes the empty π^* orbital towards ψ_2. In the process the overlap between the doubly occupied donor orbital ψ_1 and the empty acceptor orbital ψ_2 is maximized. This "chemically-induced orbital

polarization" is realized by mixing π and π* and correspondingly polarizing the π bond pair so that it becomes the lone pair on ψ_3. Resulting from this formally dative bond formation are the σ and σ* levels that are combinations of ψ_1 and ψ_2. The perturbation theory details of this mixing may be found in several places in the literature.[3,4]

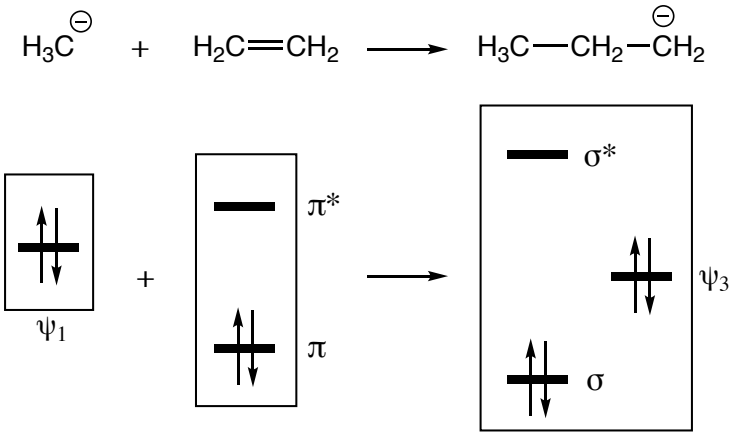

Figure S6.1. MO analysis of a typical closed-shell reaction.

Concerted pericylic reactions, which also involve decoupling and recoupling of bond pair, can be similarly analyzed, with additional considerations of orbital symmetry rules.

S6.2. Closed-shell Reactivity of Diradical(oid)s

Now, let's turn to the closed-shell reactivity of singlet diradical(oid)s, concerted pericyclic reactions that are not possible for the triplet states. Here we work with delocalized MOs. For the closed-shell singlet state (usually the lowest singlet) based on delocalized MOs, the electrons are formally paired in the two-configuration closed-shell wave function. As mentioned in the end of Section 8 and to be discussed further in Section 13, when HOMO and LUMO are close in energy and the two closed-shell configurations $|\psi_H^2\rangle$ and $|\psi_L^2\rangle$ make similar contributions to the ground state wave function, the molecule is essentially a diradical(oid) with singlet open-shell character. However, this character does not prevent the

molecule from reacting like a closed-shell molecule, which has been demonstrated above. Actually, diradical(oid)s are expected to exhibit even more active closed-shell reaction modes than regular closed-shell molecules. This is because the orbitals are easy to polarize and localize, a consequence of the small HOMO-LUMO gap. The electron pair as a donor, and the empty orbital as an acceptor, are concentrated towards the incoming species, and thus facilitate formation of dative bonds.

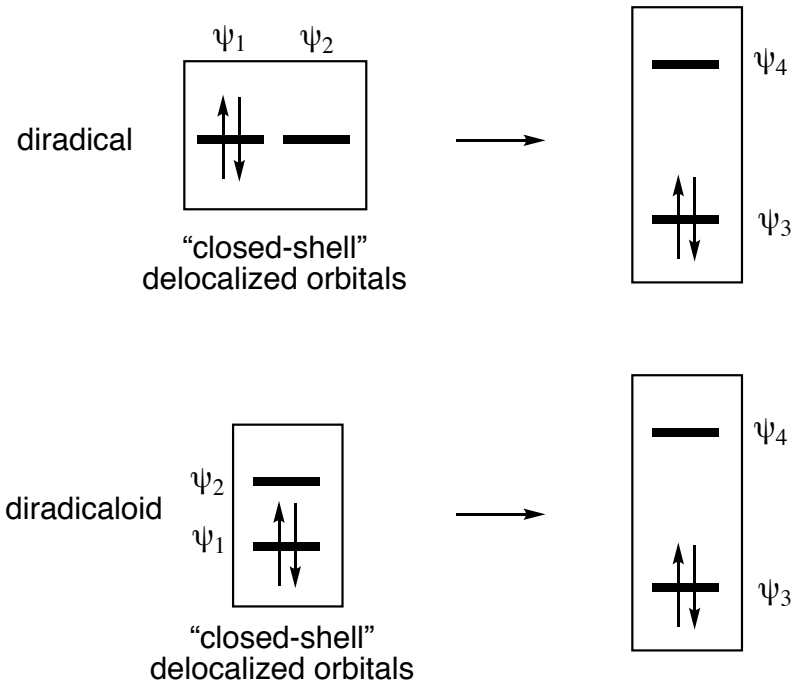

Figure S6.2. MO view of a typical closed-shell reaction of the closed-shell singlet state of a diradical (top) and a diradicaloid (bottom). A closed-shell reaction is one without unpaired spins, such as a nucleophilic/electrophilic reaction or a concerted pericyclic reaction. Only one of the two equivalent closed-shell configurations of the singlet diradical is shown.

S7. Geometries and Electronic Energies

Units:

- Coordinates are expressed in Å
- Energies are expressed in a.u.

Table 1

•CH_3

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000	0.000000	0.000454
H	0.000000	1.078131	-0.000907
H	0.933689	-0.539065	-0.000907
H	-0.933689	-0.539065	-0.000907

UB3LYP/aug-cc-pVTZ energy: -39.8594092

Transition state of the addition reaction of •CH_3 + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	-0.496390	0.639731	0.000032
H	-0.246973	1.155539	0.916627
H	-0.247148	1.155751	-0.916491
C	-1.400637	-0.366132	-0.000010
H	-1.754982	-0.808914	0.921174
H	-1.755147	-0.808691	-0.921238
C	1.652919	-0.237352	-0.000022
H	1.629641	-0.800834	0.920393
H	1.630060	-0.799817	-0.921069
H	2.209196	0.689488	0.000600

UB3LYP/aug-cc-pVTZ energy: -118.4736264

Product of the addition reaction of •CH_3 + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	-0.081506	0.550680	0.043202
H	-0.086950	1.134987	0.977252
H	-0.108276	1.303509	-0.751980
C	-1.301576	-0.293674	-0.025354
H	-1.273265	-1.334116	0.268399

H	-2.265247	0.138411	-0.254832
C	1.225705	-0.241112	-0.032381
H	1.283771	-0.974908	0.773648
H	1.302709	-0.779708	-0.977880
H	2.091515	0.416460	0.052595

UB3LYP/aug-cc-pVTZ energy: -118.52113

Ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000	-0.662394	0.000000
H	-0.920827	-1.231604	0.000000
H	0.920783	-1.231656	0.000000
C	0.000000	0.662394	0.000000
H	0.920827	1.231604	0.000000
H	-0.920783	1.231656	0.000000

UB3LYP/aug-cc-pVTZ energy: -78.6240649

ethane

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000	0.000000	0.763651
H	-0.507771	0.880282	1.161007
H	-0.508460	-0.879884	1.161007
H	1.016232	-0.000398	1.161007
C	0.000000	0.000000	-0.763651
H	0.508460	-0.879884	-1.161007
H	-1.016232	-0.000398	-1.161007
H	0.507771	0.880282	-1.161007

UB3LYP/aug-cc-pVTZ energy: -79.8647111

Transition state of the H-abstraction reaction of $\bullet CH_3 + SiH_4$

UB3LYP/aug-cc-pVTZ geometry:

C	2.118847	-0.000009	-0.000001
H	2.329778	1.053331	0.128310
H	2.330307	-0.415432	-0.976314
H	2.330186	-0.637716	0.848017
H	0.512985	-0.000483	-0.000011
H	-1.601049	0.889592	-1.079791
H	-1.601078	0.490615	1.310145
H	-1.601837	-1.379669	-0.230377
Si	-1.100884	-0.000013	0.000002

UB3LYP/aug-cc-pVTZ energy: -331.7663228

SiH4

UB3LYP/aug-cc-pVTZ geometry:

Si	0.000000	0.000000	0.000000
H	0.856376	0.856376	0.856376
H	-0.856376	-0.856376	0.856376
H	-0.856376	0.856376	-0.856376
H	0.856376	-0.856376	-0.856376

UB3LYP/aug-cc-pVTZ energy: -291.918338\RMSD=1

•SiH3

UB3LYP/aug-cc-pVTZ geometry:

Si	0.000000	0.000000	0.080338
H	0.000000	1.413675	-0.374911
H	-1.224278	-0.706837	-0.374911
H	1.224278	-0.706837	-0.374911

UB3LYP/aug-cc-pVTZ energy: -291.2651651

CH_4

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000	0.000000	0.000000
H	0.628147	0.628147	0.628147
H	-0.628147	-0.628147	0.628147
H	-0.628147	0.628147	-0.628147
H	0.628147	-0.628147	-0.628147

UB3LYP/aug-cc-pVTZ energy: -40.5384307

H•

UB3LYP/aug-cc-pVTZ geometry:

H	0.000000	0.000000	0.000000

UB3LYP/aug-cc-pVTZ energy: -0,5022597

Transition state of the addition reaction of H• + ethylene

UB3LYP/aug-cc-pVTZ geometry:

H	-1.674436	1.653021	0.000456

C	-0.539902	-0.271134	-0.000073
H	-1.078192	-0.455374	0.919954
H	-1.078207	-0.454824	-0.920200
C	0.747197	0.071771	0.000018
H	1.293540	0.226400	0.921121
H	1.293522	0.226956	-0.921002

UB3LYP/aug-cc-pVTZ energy: -79.1257021

Product of the addition reaction of H• + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	-0.691503	0.000004	-0.002205
H	-1.091887	-0.000233	1.022536
H	-1.103633	-0.884461	-0.491916
H	-1.103629	0.884683	-0.491524
C	0.791985	0.000000	-0.017041
H	1.348119	-0.924379	0.038190
H	1.348139	0.924366	0.038191

UB3LYP/aug-cc-pVTZ energy: -79.1931426

Transition state of the H-abstraction reaction of H• + SiH_4

UB3LYP/aug-cc-pVTZ geometry:

Si	0.000000	0.000000	0.158804
H	0.000000	1.402848	0.638670
H	1.214902	-0.701424	0.638670
H	-1.214902	-0.701424	0.638670
H	0.000000	0.000000	-1.378422
H	0.000000	0.000000	-2.760838

UB3LYP/aug-cc-pVTZ energy: -292.4184951

H_2

UB3LYP/aug-cc-pVTZ geometry:

H	-0.3716000	0.000000	0.000000
H	0.3716000	0.000000	0.000000

UB3LYP/aug-cc-pVTZ energy: -1.1800238

•CH_3

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.000000000	0.000000000	0.000857936
H	0.000000000	2.037372324	-0.001713982
H	1.764416502	-1.018685217	-0.001713982
H	-1.764416502	-1.018685217	-0.001713982

UCCSD(T)/aug-cc-pVTZ energy: -39.76178476

Transition state of the addition reaction of •CH_3 + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.938041154	1.208916388	0.000060471
H	-0.466711332	2.183652244	1.732173995
H	-0.467042034	2.184052866	-1.731916992
C	-2.646820340	-0.691889208	-0.000018897
H	-3.316435346	-1.528625924	1.740766579
H	-3.316747150	-1.528204515	-1.740887522
C	3.123564227	-0.448530277	-0.000041574
H	3.079575183	-1.513356937	1.739290703
H	3.080366978	-1.511435085	-1.740568158
H	4.174775411	1.302943491	0.001133836

UCCSD(T)/aug-cc-pVTZ energy: -118.19190120

Product of the addition reaction of •CH_3 + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.154024018	1.040634386	0.081639948
H	-0.164311687	2.144814593	1.846738641
H	-0.204611987	2.463275020	-1.421036256
C	-2.459622179	-0.554963432	-0.047912116
H	-2.406122143	-2.521113868	0.507200604
H	-4.280696450	0.261558884	-0.481562690
C	2.316246768	-0.455635647	-0.061191222
H	2.425975605	-1.842309123	1.461982842
H	2.461763239	-1.473434582	-1.847925389
H	3.952390550	0.786995345	0.099390146

UCCSD(T)/aug-cc-pVTZ energy: -118.24456588

Transition state of the H-abstraction reaction of •CH_3 + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	4.004040544	-0.000017008	-0.000001890
H	4.402642367	1.990507116	0.242470760
H	4.403642032	-0.785052706	-1.844966078
H	4.403413375	-1.205108590	1.602519885
H	0.969401160	-0.000912738	-0.000020787

H	-3.025544133	1.681085249	-2.040509269
H	-3.025598935	0.927127986	2.475815242
H	-3.027033237	-2.607196562	-0.435349437
Si	-2.080369262	-0.000024566	0.000003779

UCCSD(T)/aug-cc-pVTZ energy: -331.18662230

ethane

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.000000000	0.000000000	1.443091250
C	0.000000000	0.000000000	-1.443091250
H	-0.959548127	1.663491898	2.193985267
H	0.959548127	1.663491898	-2.193985267
H	-0.960850149	-1.662739787	2.193985267
H	0.960850149	-1.662739787	-2.193985267
H	1.920400166	-0.000752111	2.193985267
H	-1.920400166	-0.000752111	-2.193985267

UCCSD(T)/aug-cc-pVTZ energy: -79.67640102

SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	0.000000000	0.000000000	0.000000000
H	1.618316106	1.618316106	1.618316106
H	-1.618316106	-1.618316106	1.618316106
H	-1.618316106	1.618316106	-1.618316106
H	1.618316106	-1.618316106	-1.618316106

UCCSD(T)/aug-cc-pVTZ energy: -291.43922702

•SiH_3

UCCSD(T)/aug-cc-pVTZ geometry:

Si	0.000000000	0.000000000	0.151816818
H	0.000000000	2.671458589	-0.708479114
H	-2.313550129	-1.335728350	-0.708479114
H	2.313550129	-1.335728350	-0.708479114

UCCSD(T)/aug-cc-pVTZ energy: -290.78803126

Transition state of the H-abstraction reaction of H + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

H	1.353978720	1.133260390	2.345134539

H	1.353978720	1.133260390	-2.345134539
H	-2.707881378	1.133496681	0.000000000
H	0.000101403	-2.532607182	0.000000000
H	-0.000205697	-4.063285311	0.000000000
Si	0.000000000	0.513744726	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -291.92276655

Product of the addition reaction of H• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.306751289	0.000007559	-0.004166846
H	-2.063367396	-0.000440306	1.932313000
H	-2.085564120	-1.671389064	-0.929586520
H	-2.085556561	1.671808583	-0.928845747
C	1.496634750	0.000000000	-0.032202823
H	2.547575703	-1.746823152	0.072168641
H	2.547613497	1.746798585	0.072170531

UCCSD(T)/aug-cc-pVTZ energy: -79.00434178

Transition state of the addition reaction of H• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

H	-3.164225465	3.123756979	0.000861715
C	-1.020266918	-0.512369005	-0.000137950
H	-2.037487597	-0.860532147	1.738461114
H	-2.037515943	-0.859492798	-1.738925986
C	1.411997696	0.135627534	0.000034015
H	2.444436340	0.427833996	1.740666424
H	2.444402325	0.428884684	-1.740441546

UCCSD(T)/aug-cc-pVTZ energy: -78.93765730

H_2

UCCSD(T)/aug-cc-pVTZ geometry:

H	0.000000000	0.000000000	0.701904756
H	0.000000000	0.000000000	-0.701904756

UCCSD(T)/aug-cc-pVTZ energy: -1.17245621

ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	1.251195231	-0.000015118	0.000183303

C	-1.251503256	-0.000011338	-0.000177634
H	2.327377255	1.739878408	-0.000289128
H	2.327526543	-1.739799040	-0.000306136
H	-2.326445620	1.740509577	0.000274010
H	-2.326611916	-1.740430208	0.000292908

UCCSD(T)/aug-cc-pVTZ energy: -78.44054096

H radical

UCCSD(T)/aug-cc-pVTZ geometry:

H	0.000000000	0.000000000	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -0.49980991

Table 2

^{3}•CH_2-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000000	0.000000000	-1.280478408
H	0.000000000	1.747174943	-2.298632215
H	0.000000000	-1.747174943	-2.298632215
C	0.000000000	0.000000000	1.280478408
H	1.747174943	0.000000000	2.298632215
H	-1.747174943	0.000000000	2.298632215

UB3LYP/aug-cc-pVTZ energy: -78.45233175

ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000000	0.000000000	-1.280478408
C	0.000000000	0.000000000	1.280478408
H	-1.235439242	1.235439242	-2.298632215
H	1.235439242	-1.235439242	-2.298632215
H	1.235439242	-1.235439242	2.298632215
H	-1.235439242	1.235439242	2.298632215

UB3LYP/aug-cc-pVTZ energy: -78.40490855

^{3}•CH_2-CH_2-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	0.000211649	0.998075864	-0.002804354
H	0.035383232	2.297523361	-1.638411453

H	-0.034275853	2.308869277	1.622908140
C	-2.359657557	-0.527777832	-0.010470972
H	-2.347196702	-2.461466552	-0.666803094
H	-4.161186390	0.335844018	0.411941399
C	2.359778499	-0.528420339	0.014821122
H	2.340393688	-2.469577256	0.648336690
H	4.164884584	0.337537212	-0.387242679

UB3LYP/aug-cc-pVTZ energy: -117.75697560

^{3}•CH_2-CH_2-CH_2• (optimal coupling)

UB3LYP/aug-cc-pVTZ geometry:

C	0.000211649	0.998075864	-0.002804354
H	0.035383232	2.297523361	-1.638411453
H	-0.034275853	2.308869277	1.622908140
C	-2.359657557	-0.527777832	-0.010470972
H	-3.224639537	-1.098880054	-1.769938962
H	-3.374369039	-0.887635072	1.724649899
C	2.359778499	-0.528420339	0.014821122
H	3.349233829	-0.897306690	1.762593691
H	3.244622691	-1.100503348	-1.734383708

UB3LYP/aug-cc-pVTZ energy: -117.75212584

^{3}•CH_2-CH_2-CH_2-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	-3.635434345	0.264178044	-0.044499271
H	-3.953830521	2.166058894	0.634290355
H	-5.259187192	-0.805503322	-0.666648136
C	-1.106032138	-0.928658664	0.183069109
H	-0.894770205	-1.810905654	2.055763139
H	-0.928911887	-2.483685952	-1.168553727
C	1.106020800	0.928630318	-0.183074778
H	0.928877872	2.483642488	1.168570735
H	0.894749418	1.810865970	-2.055759359
C	3.635438124	-0.264155367	0.044503050
H	3.953968471	-2.165981415	-0.634381062
H	5.259149398	0.805546786	0.666733174

UB3LYP/aug-cc-pVTZ energy: -157.05587508

^{3}•CH_2-CH_2-CH_2-CH_2• (optimal coupling)

UB3LYP/aug-cc-pVTZ geometry:

C	-3.635434345	0.264178044	-0.044499271

H	-4.576776851	0.369987457	-1.856117579
H	-4.484313817	1.255772374	1.525215686
C	-1.106032138	-0.928658664	0.183069109
H	-0.894770205	-1.810905654	2.055763139
H	-0.928911887	-2.483685952	-1.168553727
C	1.106020800	0.928630318	-0.183074778
H	0.928877872	2.483642488	1.168570735
H	0.894749418	1.810865970	-2.055759359
C	3.635438124	-0.264155367	0.044503050
H	4.472930674	-0.585448229	1.881529085
H	4.587289000	-1.048328482	-1.582433872

UB3LYP/aug-cc-pVTZ energy: -157.05433344

^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	6.017628775	0.427093224	0.038382227
H	6.140096256	2.368828398	-0.587589554
H	7.757686707	-0.528339080	0.517724489
C	3.584840707	-0.968624482	-0.076454540
H	3.477697015	-2.059261022	-1.849074343
H	3.523180833	-2.398066240	1.420786812
C	1.243248932	0.727130711	0.095552112
H	1.329214464	2.144419640	-1.409096967
H	1.297614463	1.774815665	1.877008275
C	-3.584846376	0.968658497	0.076018013
H	-3.523280988	2.397459638	-1.421829941
H	-3.477655441	2.060083052	1.848161605
C	-6.017621216	-0.427132908	-0.038140343
H	-6.140030116	-2.368641315	0.588541976
H	-7.757720722	0.528051842	-0.517817085
C	-1.243252712	-0.727130711	-0.095344242
H	-1.329382649	-2.144053033	1.409643097
H	-1.297417932	-1.775265420	-1.876541512

UB3LYP/aug-cc-pVTZ energy: -235.65310921

^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$• (optimal coupling)

UB3LYP/aug-cc-pVTZ geometry:

C	6.017628775	0.427093224	0.038382227
H	7.034811584	0.898408136	-1.670528483
H	6.940561739	0.788472014	1.823885408
C	3.584840707	-0.968624482	-0.076454540
H	3.477697015	-2.059261022	-1.849074343
H	3.523180833	-2.398066240	1.420786812
C	1.243248932	0.727130711	0.095552112

H	1.329214464	2.144419640	-1.409096967
H	1.297614463	1.774815665	1.877008275
C	-3.584846376	0.968658497	0.076018013
H	-3.523280988	2.397459638	-1.421829941
H	-3.477655441	2.060083052	1.848161605
C	-6.017621216	-0.427132908	-0.038140343
H	-6.913362703	-1.109032456	1.667681969
H	-7.061346533	-0.581913440	-1.786595216
C	-1.243252712	-0.727130711	-0.095344242
H	-1.329382649	-2.144053033	1.409643097
H	-1.297417932	-1.775265420	-1.876541512

UB3LYP/aug-cc-pVTZ energy: -235.65113666

^{3}•CH_2-(CH_2-CH_2-)$_3$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	-1.188365616	0.821683158	0.013549336
H	-1.159105097	2.064924531	-1.640766052
H	-1.154046300	2.068777682	1.664686205
C	1.188363726	-0.821700165	0.013500203
H	1.159093758	-2.064858390	-1.640879436
H	1.154059528	-2.068877838	1.664574711
C	6.023643773	-0.951118059	0.021994522
H	5.938863100	-2.228569145	-1.622501849
H	5.996717066	-2.212638753	1.664302591
C	8.424487911	0.502576444	-0.022780649
H	8.502327620	2.368310613	-0.853655434
H	10.186177538	-0.355739055	0.552017349
C	-6.023645663	0.951138846	0.021983184
H	-5.938823416	2.228616388	-1.622465944
H	-5.996709507	2.212614187	1.664342275
C	-8.424495470	-0.502544319	-0.022831671
H	-8.502242582	-2.368425886	-0.853381424
H	-10.186202105	0.355729606	0.551973885
C	-3.643758588	-0.699580393	0.020135032
H	-3.682694505	-1.941068101	1.672609827
H	-3.687985739	-1.941548091	-1.633806191
C	3.643756699	0.699569055	0.020136922
H	3.682662380	1.941049203	1.672619276
H	3.687976290	1.941561319	-1.633791073

UB3LYP/aug-cc-pVTZ energy: -314.25021659

^{3}•CH_2-(CH_2-CH_2-)$_3$$CH_2$• (optimal coupling)

UB3LYP/aug-cc-pVTZ geometry:

C	-1.187345882	0.822884853	0.021497506

C	1.187345882	-0.822884853	-0.021497506
H	-1.156658430	2.095343358	-1.610425384
H	1.156658430	-2.095343358	1.610425384
H	-1.151399323	2.040344391	1.694571204
H	1.151399323	-2.040344391	-1.694571204
C	6.022484219	-0.958621028	-0.002202967
C	-6.022484219	0.958621028	0.002202967
H	5.936039490	-2.206488677	-1.669173568
H	-5.936039490	2.206488677	1.669173568
H	5.994107430	-2.249145050	1.617388911
H	-5.994107430	2.249145050	-1.617388911
C	8.425106853	0.492697447	-0.021286234
C	-8.425106853	-0.492697447	0.021286234
H	9.303488692	1.038565892	-1.784195453
H	-9.303488692	-1.038565892	1.784195453
H	9.467050630	0.827278561	1.702969336
H	-9.467050630	-0.827278561	-1.702969336
C	-3.644602464	-0.695245210	0.001198861
C	3.644602464	0.695245210	-0.001198861
H	-3.684963254	-1.965905716	1.631313453
H	3.684963254	1.965905716	-1.631313453
H	-3.690450735	-1.907516675	-1.674586688
H	3.690450735	1.907516675	1.674586688

UB3LYP/aug-cc-pVTZ energy: -314.24858864

^{1}•CH_2-CH_2• (D_{2d} geometry)

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.0000000000	-0.7260999858
H	0.9220621340	0.0000000000	-1.2920332119
H	-0.9220621340	0.0000000000	-1.2920332119
C	0.0000000000	0.0000000000	0.7260999858
H	0.0000000000	-0.9220621340	1.2920332119
H	0.0000000000	0.9220621340	1.2920332119

(2/2)CASPT2/aug-cc-pVTZ energy: -78.29277705

^{3}•CH_2-CH_2•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.0000000000	-0.7252046396
H	0.9218944830	0.0000000000	-1.2894630722
H	-0.9218944830	0.0000000000	-1.2894630722
C	0.0000000000	0.0000000000	0.7252046396
H	0.0000000000	-0.9218944830	1.2894630722
H	0.0000000000	0.9218944830	1.2894630722

(2/2)CASPT2/aug-cc-pVTZ energy: -78.29262122

^{1}•CH_2-CH_2-CH_2• (C_{2v} geometry)

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	0.000223158	1.016862425	-0.001350398
H	-0.402579205	1.627561496	-1.944612887
H	0.297143466	2.794164724	1.030122539
C	-2.216446665	-0.325665915	1.087601715
H	-2.016608769	-2.224980649	1.797728367
H	-3.962791130	0.661385551	1.442256010
C	2.345212207	-0.533273458	0.013599490
H	2.320389917	-2.422335785	0.776609259
H	4.144219692	0.292793373	-0.466911624

(2/2)CASPT2/aug-cc-pVTZ energy: -117.51158525

^{3}•CH_2-CH_2-CH_2•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	0.0001180885	0.5381004193	-0.0007145969
H	0.0191561436	1.2140850751	-0.8667500892
H	-0.0184301629	1.2159319200	0.8637943891
C	-1.2412870029	-0.2814173800	-0.0070461083
H	-1.2298897200	-1.2796982833	-0.4143236116
H	-2.1925052736	0.1558827218	0.2498705451
C	1.2410328549	-0.2821961621	0.0071965358
H	1.2278974634	-1.2818448863	0.4109639235
H	2.1930266088	0.1549395755	-0.2470789875

(2/2)CASPT2/aug-cc-pVTZ energy: -117.51311848

^{1}•CH_2-(CH_2-CH_2-)$_2$$CH_2$•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	3.1850150167	0.2366129871	0.0414178182
H	3.2611745942	1.2399649320	-0.3883541450
H	4.1126119496	-0.2671832572	0.3245555072
C	1.8944641188	-0.5177389605	-0.0442859802
H	1.8435242905	-1.0775503069	-1.0040458455
H	1.8559236361	-1.2894267377	0.7477749692
C	0.6583420428	0.3853342768	0.0566865666
H	0.7050773114	1.1518675823	-0.7409403252
H	0.6860231484	0.9328912717	1.0176785412
C	-1.8944655473	0.5177379842	0.0443288119
H	-1.8559231395	1.2894968003	-0.7476628074
H	-1.8435326581	1.0774629399	1.0041393156

C	-3.1850136522	-0.2366106669	-0.0414492104
H	-3.2611730984	-1.2399979977	0.3882402042
H	-4.1126107146	0.2672071052	-0.3245481235
C	-0.6583408977	-0.3853235442	-0.0567162380
H	-0.7050538224	-1.1518938670	0.7408765854
H	-0.6860425784	-0.9328365413	-1.0177326444

(2/2)CASPT2/aug-cc-pVTZ energy: -235.17739521

^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	3.1852053767	0.2366365792	0.0413942370
H	3.2612519512	1.2400454352	-0.3882681033
H	4.1130279161	-0.2677847917	0.3226884622
C	1.8944489083	-0.5174435504	-0.0434593269
H	1.8433181726	-1.0776346283	-1.0030199450
H	1.8560808714	-1.2888922560	0.7488446296
C	0.6582453418	0.3854437864	0.0572277569
H	0.7052463464	1.1523051576	-0.7400698712
H	0.6851939625	0.9325886868	1.0184641238
C	-1.8944506962	0.5174427267	0.0435080076
H	-1.8560828127	1.2889711212	-0.7487182863
H	-1.8433255286	1.0775369370	1.0031253312
C	-3.1852036056	-0.2366347399	-0.0414257162
H	-3.2612495284	-1.2400822098	0.3881466266
H	-4.1130261707	0.2678085436	-0.3226802887
C	-0.6582443217	-0.3854315243	-0.0572627518
H	-0.7052192562	-1.1523357505	0.7399954463
H	-0.6852169269	-0.9325255228	-1.0185273317

(2/2)CASPT2/aug-cc-pVTZ energy: -235.17738643

^{1}•CH_2-(CH_2-CH_2-)$_3$$CH_2$•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	-0.6280760938	0.4378260017	0.0184123649
H	-0.6102459133	1.1027428659	-0.8670592389
H	-0.6103812830	1.1010650150	0.9049945300
C	0.6280778640	-0.4378246136	0.0184120686
H	0.6102617263	-1.1027202185	-0.8670757913
H	0.6103688597	-1.1010861467	0.9049773781
C	3.1851625805	-0.5089636508	0.0120406853
H	3.1407636296	-1.1786678477	-0.8751089573
H	3.1702495834	-1.1832073847	0.8893128675
C	4.4579304291	0.2792163686	-0.0039125747
H	4.5081445717	1.2252606250	-0.5511198078
H	5.3985018727	-0.1646530838	0.3320431099

C	-3.1851621168	0.5089605103	0.0120429392
H	-3.1407963175	1.1786725402	-0.8751021690
H	-3.1702245727	1.1832010786	0.8893178385
C	-4.4579267999	-0.2792254913	-0.0038724812
H	-4.5081271132	-1.2253216450	-0.5509901693
H	-5.3985023520	0.1646610398	0.3320494096
C	-1.9278073726	-0.3706516652	0.0179337804
H	-1.9519878270	-1.0328825255	0.9038494378
H	-1.9468394240	-1.0339699413	-0.8684523042
C	1.9278100990	0.3706521537	0.0179724307
H	1.9519908929	1.0328430423	0.9039179730
H	1.9468440768	1.0340109729	-0.8683833198

(2/2)CASPT2/aug-cc-pVTZ energy: -313.62100539

^{3}•CH_2-(CH_2-CH_2-)$_3$$CH_2$•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	-0.6280772156	0.4378164916	0.0182996917
H	-0.6102859138	1.1026804635	-0.8672118991
H	-0.6103462427	1.1011119546	0.9048397796
C	0.6280793012	-0.4378291509	0.0183066705
H	0.6103018845	-1.1026882906	-0.8672087333
H	0.6103371036	-1.1011290698	0.9048430118
C	3.1851569047	-0.5089591443	0.0120239361
H	3.1408285099	-1.1785949311	-0.8751782246
H	3.1701869250	-1.1832918574	0.8892319195
C	4.4579413638	0.2792015802	-0.0037718321
H	4.5080315720	1.2256283799	-0.5503204401
H	5.3985909132	-0.1649393288	0.3315995581
C	-3.1851522944	0.5089581070	0.0120327497
H	-3.1408425727	1.1786067984	-0.8751604629
H	-3.1701554120	1.1832793384	0.8892494894
C	-4.4579405187	-0.2791966136	-0.0037404072
H	-4.5080318045	-1.2256538499	-0.5502344614
H	-5.3985863143	0.1649592675	0.3316219164
C	-1.9278101255	-0.3706560826	0.0179299236
H	-1.9519506926	-1.0328223767	0.9038953479
H	-1.9468828758	-1.0340369025	-0.8684081618
C	1.9278099737	0.3706480324	0.0179616044
H	1.9519515794	1.0327826027	0.9039506502
H	1.9468749517	1.0340625818	-0.8683516266

(2/2)CASPT2/aug-cc-pVTZ energy: -313.62098911

Table 3

^{3}•CH_2-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	-0.721544	0.000003	-0.000015
H	-1.294037	0.784883	0.484280
H	-1.294064	-0.784909	-0.484214
C	0.721544	0.000012	0.000014
H	1.294035	0.484216	-0.784925
H	1.294067	-0.484278	0.784866

UB3LYP/aug-cc-pVTZ energy: -78.5201043

^{3}•CH_2-CH_2-CH_2-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	-1.923789	0.139797	-0.023548
H	-2.092277	1.146229	0.335652
H	-2.783042	-0.426254	-0.352775
C	-0.585287	-0.491425	0.096876
H	-0.473492	-0.958290	1.087863
H	-0.491559	-1.314310	-0.618372
C	0.585281	0.491410	-0.096879
H	0.491541	1.314287	0.618381
H	0.473481	0.958269	-1.087861
C	1.923791	-0.139785	0.023550
H	2.092350	-1.146188	-0.335700
H	2.783022	0.426277	0.352820

UB3LYP/aug-cc-pVTZ energy: -157.1754656

^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	3.184392	0.226008	0.020311
H	3.249199	1.253530	-0.310939
H	4.105191	-0.279585	0.273968
C	1.897016	-0.512574	-0.040458
H	1.840318	-1.089714	-0.978488
H	1.864387	-1.269002	0.751848
C	0.657899	0.384781	0.050564
H	0.703390	1.134778	-0.745662
H	0.686668	0.939192	0.993270
C	-1.897019	0.512592	0.040227
H	-1.864440	1.268681	-0.752400
H	-1.840296	1.090149	0.978005
C	-3.184388	-0.226029	-0.020183
H	-3.249164	-1.253431	0.311443
H	-4.105209	0.279433	-0.274017
C	-0.657901	-0.384781	-0.050454

H	-0.703479	-1.134584	0.745951
H	-0.686564	-0.939430	-0.993023

UB3LYP/aug-cc-pVTZ energy: -235.8312014

^{3}•CH_2-(CH_2-CH_2-)$_3$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	-0.628856	0.434816	0.007170
H	-0.613372	1.092711	-0.868256
H	-0.610695	1.094750	0.880914
C	0.628855	-0.434825	0.007144
H	0.613366	-1.092676	-0.868316
H	0.610702	-1.094803	0.880855
C	3.187575	-0.503310	0.011639
H	3.142711	-1.179308	-0.858591
H	3.173326	-1.170878	0.880711
C	4.458047	0.265952	-0.012055
H	4.499238	1.253256	-0.451735
H	5.390293	-0.188249	0.292115
C	-3.187576	0.503321	0.011633
H	-3.142690	1.179333	-0.858572
H	-3.173322	1.170865	0.880732
C	-4.458051	-0.265935	-0.012082
H	-4.499193	-1.253317	-0.451590
H	-5.390306	0.188244	0.292092
C	-1.928194	-0.370202	0.010655
H	-1.948798	-1.027169	0.885107
H	-1.951598	-1.027423	-0.864573
C	1.928193	0.370196	0.010656
H	1.948781	1.027159	0.885112
H	1.951593	1.027430	-0.864565

UB3LYP/aug-cc-pVTZ energy: -314.4868512

^{3}•CH_2-(CH_2-CH_2-)$_4$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	-1.912782	0.448442	-0.024936
H	-1.905871	1.046317	-0.942555
H	-1.898802	1.165656	0.802588
C	-0.646551	-0.407232	0.029209
H	-0.659667	-1.123470	-0.799072
H	-0.654783	-1.006113	0.945985
C	1.912785	-0.448538	0.024831
H	1.898792	-1.165824	-0.802634
H	1.905890	-1.046356	0.942492
C	-4.472415	0.492472	-0.018625

H	-4.435052	1.109632	-0.931876
H	-4.464267	1.216511	0.804129
C	-5.735204	-0.289182	0.010726
H	-5.765733	-1.305789	-0.357137
H	-6.672426	0.176117	0.280996
C	-3.204353	-0.366614	0.036542
H	-3.216903	-0.963153	0.953463
H	-3.223139	-1.081665	-0.792200
C	0.646546	0.407117	-0.029382
H	0.659634	1.123401	0.798860
H	0.654806	1.005951	-0.946191
C	3.204333	0.366540	-0.036739
H	3.222886	1.081955	0.791705
H	3.216952	0.962784	-0.953859
C	4.472450	-0.492366	0.018975
H	4.435082	-1.109084	0.932533
H	4.464518	-1.216888	-0.803330
C	5.735176	0.289363	-0.010641
H	5.765764	1.305991	0.357134
H	6.672416	-0.175983	-0.280790

UB3LYP/aug-cc-pVTZ energy: -393.14259074

Transition state of the addition reaction of ^{3}•CH_2-CH_2• + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	-0.952308	-0.598020	0.000321
H	-0.598381	-1.051208	-0.915615
H	-0.598709	-1.050315	0.916838
C	-2.069399	0.168500	-0.000254
H	-2.517225	0.515962	-0.921703
H	-2.517555	0.516868	0.920693
C	0.944563	0.679285	0.000106
H	0.744025	1.246747	-0.905415
H	0.744147	1.246549	0.905774
C	2.042248	-0.272958	-0.000141
H	3.075913	0.058414	-0.000284
H	1.877160	-1.343858	-0.000480

UB3LYP/aug-cc-pVTZ energy: -157.1320183

Transition state of the addition reaction of ^{3}•CH_2-CH_2-CH_2-CH_2• + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	1.904658	-0.633871	-0.315685
H	1.317544	-1.337106	0.258018
H	1.583269	-0.473853	-1.335958
C	3.175567	-0.344382	0.057079

H	3.559528	-0.628206	1.027778
H	3.830719	0.242412	-0.572896
C	0.480373	1.052344	0.302219
H	0.586021	0.957556	1.376295
C	-0.861916	0.776412	-0.297055
H	-1.472434	1.691053	-0.244743
H	-0.764276	0.565629	-1.367089
C	-1.644907	-0.359578	0.376703
H	-1.092575	-1.299552	0.288424
H	-1.681205	-0.152629	1.459143
C	-3.021911	-0.533433	-0.151974
H	-3.582792	0.315493	-0.519148
H	-3.539033	-1.477938	-0.063712
H	1.064053	1.852184	-0.133829

UB3LYP/aug-cc-pVTZ energy: -235.7865347

Transition state of the addition reaction of $^{3}\bullet CH_2\text{-}(CH_2\text{-}CH_2\text{-})_2CH_2\bullet$ + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	2.925483	-0.814994	-0.401135
H	2.168744	-1.420372	0.077538
H	2.693609	-0.475333	-1.401490
C	4.212414	-0.872102	0.022119
H	4.479834	-1.341382	0.959404
H	5.010647	-0.388865	-0.525380
C	1.900460	1.076363	0.385144
H	1.967015	0.857047	1.443934
C	0.538170	1.162815	-0.227125
H	0.148956	2.183463	-0.087353
H	0.606582	1.038078	-1.314126
C	-0.483735	0.174126	0.340644
H	-0.140165	-0.848854	0.163324
H	-0.530494	0.295345	1.427845
H	2.654212	1.763975	0.024588
C	-1.883308	0.344178	-0.248915
H	-1.838957	0.233187	-1.336317
H	-2.235651	1.363442	-0.060613
C	-2.906372	-0.648674	0.313862
H	-2.568219	-1.674078	0.126720
H	-2.913897	-0.554206	1.412680
C	-4.281558	-0.466953	-0.217295
H	-4.622108	0.503881	-0.550905
H	-5.009441	-1.263889	-0.163636

UB3LYP/aug-cc-pVTZ energy: -314.4422168

Transition state of the addition reaction of $^{3}\bullet CH_2\text{-}(CH_2\text{-}CH_2\text{-})_3CH_2\bullet$ + ethylene

UB3LYP/aug-cc-pVTZ geometry:

C	4.048232	-0.978090	-0.475383
H	3.197494	-1.506800	-0.069317
H	3.906722	-0.540101	-1.454092
C	5.296506	-1.239897	-0.015205
H	5.457930	-1.806235	0.892246
H	6.175083	-0.832639	-0.497544
C	3.245133	0.973454	0.412295
H	3.288766	0.699942	1.459488
C	1.900117	1.233368	-0.189577
H	1.639093	2.292286	-0.038511
H	1.947226	1.112299	-1.278465
C	0.768190	0.370824	0.374848
H	0.997380	-0.686242	0.212696
H	0.724129	0.508558	1.460040
H	4.070358	1.588169	0.077437
C	-0.598293	0.687994	-0.232972
H	-0.551496	0.549187	-1.318226
H	-0.827219	1.747101	-0.074085
C	-1.733958	-0.163663	0.335322
H	-1.503567	-1.222857	0.178920
H	-1.783198	-0.022655	1.420281
C	-3.098786	0.151237	-0.276451
H	-3.056046	0.007829	-1.360066
H	-3.332995	1.208921	-0.118327
C	-4.236272	-0.701553	0.296635
H	-4.014426	-1.763889	0.144674
H	-4.248082	-0.573587	1.392054
C	-5.574303	-0.380892	-0.262971
H	-5.798068	0.612889	-0.626562
H	-6.388485	-1.088870	-0.201888

UB3LYP/aug-cc-pVTZ energy: -393.0978521\S2

Transition state of the H-abstraction reaction of $^{3}\bullet CH_2\text{-}CH_2\bullet + SiH_4$

UB3LYP/aug-cc-pVTZ geometry:

C	-1.453257	0.695299	0.000553
H	-1.497461	1.304260	-0.902795
H	-1.499641	1.303996	0.904061
H	0.067239	0.341530	-0.000962
H	2.147692	-0.155891	-1.397297
H	1.839507	-1.378692	0.671635
H	2.421417	0.971294	0.729884
Si	1.649023	-0.066999	-0.000361
C	-2.161036	-0.579223	-0.000704
H	-3.244478	-0.619435	-0.005253
H	-1.634847	-1.525541	0.006694

UB3LYP/aug-cc-pVTZ energy: -370.4249424

Transition state of the H-abstraction reaction of ^{3}•CH_2-CH_2-CH_2-CH_2• + SiH_4

UB3LYP/aug-cc-pVTZ geometry:

H	-2.339344	-1.341706	1.253568
H	-2.585019	-1.375233	-1.153754
H	-3.765026	0.279711	0.160490
H	-1.240775	0.537282	-0.104237
C	-0.046099	1.550550	-0.195656
H	-0.028662	1.732841	-1.266147
H	-0.477227	2.364780	0.377362
C	1.139614	0.852282	0.399780
H	0.895555	0.497008	1.406508
H	1.959008	1.570693	0.536990
C	1.656233	-0.322214	-0.442179
H	1.903285	0.030581	-1.449288
H	0.827193	-1.033353	-0.590106
C	2.823415	-1.021706	0.151466
H	2.954961	-1.065079	1.224142
H	3.489224	-1.612232	-0.461107
Si	-2.502297	-0.495626	0.041794

UB3LYP/aug-cc-pVTZ energy: -449.0805563

Transition state of the H-abstraction reaction of ^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$• + SiH_4

UB3LYP/aug-cc-pVTZ geometry:

H	-3.216863	-1.940640	-1.143224
H	-4.747579	-0.787498	0.334598
H	-2.779222	-1.868312	1.235134
H	-2.477709	0.288628	-0.126649
C	-1.702187	1.641694	-0.291800
H	-1.706406	1.733364	-1.373925
H	-2.412141	2.296349	0.203225
C	-0.371469	1.449971	0.372882
H	-0.518249	1.116062	1.405811
H	0.135826	2.422173	0.455359
C	0.554218	0.473023	-0.356444
H	0.684943	0.810220	-1.389958
H	0.070877	-0.506964	-0.416436
C	1.922857	0.324407	0.305941
H	1.792798	-0.012072	1.339525
H	2.409431	1.302568	0.362763
C	2.849906	-0.654338	-0.423177
H	2.983324	-0.332371	-1.462315
H	2.338292	-1.628376	-0.497665

C	4.175221	-0.828358	0.224385
H	4.295870	-0.677057	1.288463
H	5.014194	-1.231641	-0.324496
Si	-3.317048	-1.101631	0.079933

UB3LYP/aug-cc-pVTZ energy: -527.7362774

Transition state of the H-abstraction reaction of ^{3}•CH_2-(CH_2-CH_2-)$_3$$CH_2$• + SiH_4

UB3LYP/aug-cc-pVTZ geometry:

H	3.393442	-2.230846	-1.069185
H	4.314002	-2.230022	1.167535
H	5.633608	-1.401703	-0.684378
H	3.674215	0.020417	0.136273
C	3.138608	1.479595	0.343457
H	3.145099	1.535064	1.428020
H	3.955450	2.019064	-0.125003
C	1.803100	1.535177	-0.337152
H	1.903332	1.200932	-1.375653
H	1.473288	2.582114	-0.403870
C	0.713061	0.719670	0.362676
H	0.619137	1.064297	1.397648
H	1.025577	-0.327504	0.419247
C	-0.648665	0.804439	-0.326671
H	-0.551859	0.457697	-1.360784
H	-0.957899	1.853285	-0.387490
C	-1.740687	-0.003315	0.375580
H	-1.840172	0.345766	1.408868
H	-1.429136	-1.051223	0.439653
Si	4.261422	-1.486228	-0.118549
C	-3.100689	0.076531	-0.317305
H	-3.007090	-0.276782	-1.348357
H	-3.415894	1.123021	-0.381353
C	-4.194591	-0.730500	0.390415
H	-3.888137	-1.780056	0.467174
H	-4.262238	-0.384014	1.435190
C	-5.528090	-0.641679	-0.257900
H	-6.295657	-1.374948	-0.055323
H	-5.801253	0.223127	-0.847139

UB3LYP/aug-cc-pVTZ energy: -606.3918913

CH_3-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	0.792095	-0.000100	0.000000
H	1.362677	0.916323	0.000000
H	1.338795	-0.932414	0.000000

C	-0.692026	0.005451	0.000000
H	-1.102306	-0.516399	-0.873685
H	-1.102305	-0.516396	0.873687
H	-1.097276	1.016779	-0.000002

UB3LYP/aug-cc-pVTZ energy: -79.1921398

CH_3-CH_2-CH_2-CH_2•

UB3LYP/aug-cc-pVTZ geometry:

C	0.508120	0.520884	-0.059131
H	0.403228	1.251080	0.748624
H	0.417001	1.083404	-0.991864
C	-0.643388	-0.486818	0.030056
H	-0.523196	-1.068820	0.959329
H	-0.548557	-1.226817	-0.773030
C	-1.993946	0.129862	-0.008497
H	-2.150489	1.141879	0.339673
H	-2.866526	-0.454331	-0.263841
C	1.885975	-0.132942	0.016445
H	2.682642	0.609404	-0.047333
H	2.014323	-0.677312	0.954461
H	2.031009	-0.844404	-0.799257

UB3LYP/aug-cc-pVTZ energy: -157.8479236

CH_3-(CH_2-CH_2-)$_2$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	-1.821133	0.543653	-0.034139
H	-1.785363	1.145399	-0.947302
H	-1.777771	1.253684	0.797249
C	-0.592248	-0.365117	0.016878
H	-0.635656	-1.075248	-0.815944
H	-0.628476	-0.969002	0.930075
C	1.963521	-0.517892	0.014699
H	1.927696	-1.232339	-0.815673
H	1.897616	-1.142424	0.921319
C	3.257909	0.210651	-0.002649
H	3.329814	1.220479	0.377924
H	4.175788	-0.290192	-0.275810
C	0.732915	0.394326	-0.034964
H	0.780099	1.100610	0.800183
H	0.772914	0.997963	-0.946465
C	-3.142049	-0.222296	0.019293
H	-3.997561	0.453433	-0.021473
H	-3.229049	-0.917636	-0.818284
H	-3.223543	-0.804670	0.939496

UB3LYP/aug-cc-pVTZ energy: -236.5035255

CH_3-(CH_2-CH_2-)$_3$$CH_2$•

UB3LYP/aug-cc-pVTZ geometry:

C	-0.699442	-0.427703	-0.000001
H	-0.678262	-1.086707	0.874540
H	-0.678263	-1.086704	-0.874545
C	0.552806	0.449981	-0.000001
H	0.531421	1.108948	0.874448
H	0.531420	1.108949	-0.874449
C	3.111685	0.532567	0.000001
H	3.089767	1.190726	0.873906
H	3.089768	1.190729	-0.873903
C	-3.257029	-0.510828	0.000005
H	-3.225403	-1.186300	0.867770
H	-3.225406	-1.186302	-0.867758
C	-4.533532	0.249274	0.000006
H	-4.543275	1.330113	-0.000011
H	-5.484154	-0.265005	-0.000052
C	-2.004073	0.368131	0.000002
H	-2.029730	1.025192	-0.874931
H	-2.029725	1.025192	0.874935
C	1.859021	-0.344548	-0.000002
H	1.881454	-1.003791	-0.874447
H	1.881454	-1.003794	0.874442
C	4.411681	-0.270178	0.000000
H	4.478552	-0.912454	-0.880693
H	5.285123	0.383482	0.000001
H	4.478552	-0.912457	0.880691

UB3LYP/aug-cc-pVTZ energy: -315.1

^{3}•CH_2-CH_2•

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.363520552	0.000005669	-0.000028346
H	-2.445375534	1.483213915	0.915156571
H	-2.445426557	-1.483263048	-0.915031849
C	1.363520552	0.000022677	0.000026456
H	2.445371754	0.915035628	-1.483293284
H	2.445432226	-0.915152791	1.483181790

UCCSD(T)/aug-cc-pVTZ energy: -78.33234984

CH_3-CH_2•

UCCSD(T)/aug-cc-pVTZ geometry:

C	1.496617743	-0.000005669	-0.033899797
H	2.548422300	-1.746448986	0.075367947
H	2.548125613	1.746362058	0.076341156
C	-1.307012071	0.000171965	-0.003798350
H	-2.063108504	-0.004098816	1.933125582
H	-2.085431839	1.673154068	-0.926570517
H	-2.085637819	-1.669960431	-0.932075289

UCCSD(T)/aug-cc-pVTZ energy: -79.00434672

Transition state of the H-abstraction reaction of ^{3}•CH_2-CH_2• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	-2.746257729	1.313924689	0.001045019
H	-2.829791182	2.464694204	-1.706035303
H	-2.833910785	2.464195316	1.708427696
H	0.127063295	0.645398166	-0.001817917
H	4.058549695	-0.294591296	-2.640508654
H	3.476164447	-2.605350300	1.269206210
H	4.575814980	1.835479653	1.379280868
Si	3.116201854	-0.126609761	-0.000682191
C	-4.083766200	-1.094572839	-0.001330367
H	-6.131174859	-1.170562506	-0.009926731
H	-3.089413097	-2.882854692	0.012649827

UCCSD(T)/aug-cc-pVTZ energy: -369.75626490

Transition state of the addition reaction of ^{3}•CH_2-CH_2• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.799601313	-1.130094021	0.000606602
H	-1.130776212	-1.986495227	-1.730261592
H	-1.131396042	-1.984807702	1.732572727
C	-3.910597367	0.318418853	-0.000479990
H	-4.756865861	0.975026874	-1.741766245
H	-4.757489471	0.976738966	1.739857621
C	1.784965384	1.283662615	0.000200311
H	1.406003485	2.356010385	-1.710986385
H	1.406234032	2.355636219	1.711664797
C	3.859289412	-0.515815865	-0.000266451
H	5.812633174	0.110386462	-0.000536682
H	3.547318305	-2.539523580	-0.000907069

UCCSD(T)/aug-cc-pVTZ energy: -156.76269075

^{3}•CH_2-CH_2-CH_2-CH_2•

UCCSD(T)/aug-cc-pVTZ geometry:

C	-3.635434345	0.264178044	-0.044499271
H	-3.953830521	2.166058894	0.634290355
H	-5.259187192	-0.805503322	-0.666648136
C	-1.106032138	-0.928658664	0.183069109
H	-0.894770205	-1.810905654	2.055763139
H	-0.928911887	-2.483685952	-1.168553727
C	1.106020800	0.928630318	-0.183074778
H	0.928877872	2.483642488	1.168570735
H	0.894749418	1.810865970	-2.055759359
C	3.635438124	-0.264155367	0.044503050
H	3.953968471	-2.165981415	-0.634381062
H	5.259149398	0.805546786	0.666733174

UCCSD(T)/aug-cc-pVTZ energy: -156.81288379

CH_3-CH_2-CH_2-CH_2•

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.960207642	0.984328106	-0.111741396
H	0.761990489	2.364198568	1.414694335
H	0.788017687	2.047336850	-1.874351320
C	-1.215827116	-0.919952696	0.056797609
H	-0.988697153	-2.019777084	1.812869080
H	-1.036622497	-2.318348143	-1.460814991
C	-3.768011861	0.245403615	-0.016057003
H	-4.063835259	2.157838585	0.641888944
H	-5.416949089	-0.858561163	-0.498587232
C	3.563976241	-0.251223971	0.031076546
H	5.069458689	1.151606663	-0.089446407
H	3.806518810	-1.279934186	1.803669893
H	3.838050780	-1.595692304	-1.510376839

UCCSD(T)/aug-cc-pVTZ energy: -157.48535273

Transition state of the H-abstraction reaction of ^{3}•CH_2-CH_2-CH_2-CH_2• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

H	-4.420719487	-2.535456889	2.368900207
H	-4.884977955	-2.598813737	-2.180279083
H	-7.114868018	0.528577186	0.303282147
H	-2.344724941	1.015315835	-0.196979383
C	-0.087114485	2.930114853	-0.369736256
H	-0.054163330	3.274594919	-2.392671072
H	-0.901828333	4.468786561	0.713110832
C	2.153558356	1.610579567	0.755474713

H	1.692353686	0.939209005	2.657914922
H	3.701988609	2.968179607	1.014764035
C	3.129826780	-0.608896216	-0.835597211
H	3.596687400	0.057789715	-2.738757406
H	1.563168228	-1.952754167	-1.115138729
C	5.335481105	-1.930744527	0.286229258
H	5.584067019	-2.012707618	2.313293126
H	6.593677771	-3.046676940	-0.871365947
Si	-4.728656029	-0.936597404	0.078979214

UCCSD(T)/aug-cc-pVTZ energy: -448.23823628

Transition state of the addition reaction of ^{3}•CH_2-CH_2-CH_2-CH_2• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	3.599281994	-1.197842593	-0.596558194
H	2.489797326	-2.526764149	0.487583357
H	2.991944802	-0.895452397	-2.524594743
C	6.000951942	-0.650787665	0.107863678
H	6.726533077	-1.187137294	1.942218944
H	7.239009796	0.458092291	-1.082616542
C	0.907773411	1.988641956	0.571111142
H	1.107419197	1.809518595	2.600820626
C	-1.628785188	1.467206045	-0.561352596
H	-2.782497007	3.195627044	-0.462497243
H	-1.444272329	1.068883902	-2.583423807
C	-3.108423742	-0.679503943	0.711865503
H	-2.064667528	-2.455797374	0.545042370
H	-3.177017021	-0.288427010	2.757380657
C	-5.710584184	-1.008042279	-0.287189239
H	-6.770495666	0.596195366	-0.981047542
H	-6.687803140	-2.792898059	-0.120398231
H	2.010768759	3.500120505	-0.252900158

UCCSD(T)/aug-cc-pVTZ energy: -235.24335471

^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$•

UCCSD(T)/aug-cc-pVTZ geometry:

C	6.017628775	0.427093224	0.038382227
H	6.140096256	2.368828398	-0.587589554
H	7.757686707	-0.528339080	0.517724489
C	3.584840707	-0.968624482	-0.076454540
H	3.477697015	-2.059261022	-1.849074343
H	3.523180833	-2.398066240	1.420786812
C	1.243248932	0.727130711	0.095552112
H	1.329214464	2.144419640	-1.409096967
H	1.297614463	1.774815665	1.877008275

C	-3.584846376	0.968658497	0.076018013
H	-3.523280988	2.397459638	-1.421829941
H	-3.477655441	2.060083052	1.848161605
C	-6.017621216	-0.427132908	-0.038140343
H	-6.140030116	-2.368641315	0.588541976
H	-7.757720722	0.528051842	-0.517817085
C	-1.243252712	-0.727130711	-0.095344242
H	-1.329382649	-2.144053033	1.409643097
H	-1.297417932	-1.775265420	-1.876541512

UCCSD(T)/aug-cc-pVTZ energy: -235.29442240

CH_3-(CH_2-CH_2-)$_2$$CH_2$•

UCCSD(T)/aug-cc-pVTZ geometry:

C	-3.441442619	1.027355281	-0.064513360
H	-3.373847115	2.164490421	-1.790141344
H	-3.359500314	2.369119415	1.506582269
C	-1.119186522	-0.689971136	0.031894798
H	-1.201215754	-2.031924243	-1.541910699
H	-1.187647520	-1.831148401	1.757587032
C	3.710516943	-0.978674046	0.027777084
H	3.642817505	-2.328783211	-1.541398583
H	3.585974543	-2.158868486	1.741040590
C	6.156555771	0.398072699	-0.005005885
H	6.292436529	2.306371059	0.714172858
H	7.891095703	-0.548383406	-0.521205364
C	1.385008628	0.745168146	-0.066072384
H	1.474173465	2.079851478	1.512126725
H	1.460595783	1.885876759	-1.788559643
C	-5.937612102	-0.420078560	0.036458486
H	-7.554295484	0.856864189	-0.040578089
H	-6.102018275	-1.734080728	-1.546332658
H	-6.091613443	-1.520605926	1.775390142

UCCSD(T)/aug-cc-pVTZ energy: -235.96681737

Transition state of the H-abstraction reaction of ^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

H	-6.078990072	-3.667278120	-2.160380267
H	-8.971624097	-1.488155549	0.632298584
H	-5.251968438	-3.530598008	2.334064996
H	-4.682191443	0.545427874	-0.239331925
C	-3.216667254	3.102352052	-0.551422085
H	-3.224640009	3.275583246	-2.596341975
H	-4.558285880	4.339470712	0.384039593
C	-0.701974676	2.740048089	0.704644859

H	-0.979348678	2.109051526	2.656597783
H	0.256673942	4.577243613	0.860503801
C	1.047320237	0.893883924	-0.673581541
H	1.294354686	1.531093906	-2.626639954
H	0.133938119	-0.958023118	-0.786949991
C	3.633673120	0.613040385	0.578144702
H	3.387897229	-0.022812774	2.531335396
H	4.553164723	2.461496788	0.685522721
C	5.385541840	-1.236519617	-0.799688635
H	5.637665321	-0.628090164	-2.763374868
H	4.418731495	-3.077184679	-0.940450555
C	7.890024228	-1.565369759	0.424026198
H	8.118017796	-1.279452305	2.434842200
H	9.475453430	-2.327464182	-0.613208571
Si	-6.268312285	-2.081780888	0.151051479

UCCSD(T)/aug-cc-pVTZ energy: -526.71985142

Transition state of the addition reaction of ^{3}•CH_2-(CH_2-CH_2-)$_2$$CH_2$• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	5.528361672	-1.540115459	-0.758035292
H	4.098332209	-2.684114085	0.146525585
H	5.090183315	-0.898249191	-2.648432276
C	7.960308812	-1.648033939	0.041798852
H	8.465659374	-2.534844618	1.813010809
H	9.468750571	-0.734848352	-0.992824315
C	3.591348924	2.034031288	0.727816681
H	3.717119646	1.619584112	2.728639812
C	1.016993912	2.197401892	-0.429204048
H	0.281486046	4.126147088	-0.165073247
H	1.146273856	1.961683123	-2.483338242
C	-0.914126670	0.329050452	0.643723868
H	-0.264873463	-1.604101586	0.308637631
H	-1.002488374	0.558121164	2.698236008
H	5.015733775	3.333429653	0.046464586
C	-3.558936341	0.650402160	-0.470381180
H	-3.475125097	0.440659567	-2.525273155
H	-4.224768115	2.576531976	-0.114541970
C	-5.492247116	-1.225816209	0.593113223
H	-4.853230556	-3.163548943	0.239466095
H	-5.506467305	-1.047297560	2.669578311
C	-8.090972036	-0.882413286	-0.410628040
H	-8.734518270	0.952197093	-1.041059574
H	-9.466471562	-2.388404071	-0.309227225

UCCSD(T)/aug-cc-pVTZ energy: -313.72500731

^{3}•CH_2-(CH_2-CH_2-)$_3$$CH_2$•

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.188365616	0.821683158	0.013549336
H	-1.159105097	2.064924531	-1.640766052
H	-1.154046300	2.068777682	1.664686205
C	1.188363726	-0.821700165	0.013500203
H	1.159093758	-2.064858390	-1.640879436
H	1.154059528	-2.068877838	1.664574711
C	6.023643773	-0.951118059	0.021994522
H	5.938863100	-2.228569145	-1.622501849
H	5.996717066	-2.212638753	1.664302591
C	8.424487911	0.502576444	-0.022780649
H	8.502327620	2.368310613	-0.853655434
H	10.186177538	-0.355739055	0.552017349
C	-6.023645663	0.951138846	0.021983184
H	-5.938823416	2.228616388	-1.622465944
H	-5.996709507	2.212614187	1.664342275
C	-8.424495470	-0.502544319	-0.022831671
H	-8.502242582	-2.368425886	-0.853381424
H	-10.186202105	0.355729606	0.551973885
C	-3.643758588	-0.699580393	0.020135032
H	-3.682694505	-1.941068101	1.672609827
H	-3.687985739	-1.941548091	-1.633806191
C	3.643756699	0.699569055	0.020136922
H	3.682662380	1.941049203	1.672619276
H	3.687976290	1.941561319	-1.633791073

UCCSD(T)/aug-cc-pVTZ energy: -313.77596200

Table 4

Transition state of the addition reaction of $^{1}\bullet CH_2\text{-}CH_2\bullet$ + ethylene

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	-0.9334639415	-0.6056015008	0.0000000000
H	-0.5713257541	-1.0557580000	-0.9290943955
H	-0.5713257541	-1.0557580000	0.9290943955
C	-2.0733459575	0.1608519903	0.0000000000
H	-2.5190049087	0.5149928725	-0.9340408909
H	-2.5190049087	0.5149928725	0.9340408909
C	0.9401199258	0.7056287269	0.0000000000
H	0.7367962540	1.2715341020	-0.9202873948
H	0.7367962540	1.2715341020	0.9202873948
C	2.0313276017	-0.2810138975	0.0000000000
H	3.0828061435	0.0318956741	0.0000000000
H	1.8346403058	-1.3589324321	0.0000000000

(4/4)CASPT2/aug-cc-pVTZ energy: -156.68358713

Transition state of the addition reaction of ^{3}•CH_2-CH_2• + ethylene

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	-0.9465255673	-0.6136397420	0.0000000000
H	-0.5848063945	-1.0634876991	-0.9293112174
H	-0.5848063945	-1.0634876991	0.9293112174
C	-2.0781939126	0.1635573326	0.0000000000
H	-2.5209552576	0.5211710189	-0.9340817638
H	-2.5209552576	0.5211710189	0.9340817638
C	0.9385857365	0.6973191635	0.0000000000
H	0.7459063976	1.2696904809	-0.9184587886
H	0.7459063976	1.2696904809	0.9184587886
C	2.0399380509	-0.2779214530	0.0000000000
H	3.0868933513	0.0471773323	0.0000000000
H	1.8540281100	-1.3568737249	0.0000000000

(4/4)CASPT2/aug-cc-pVTZ energy: -156.68355463

Transition state of the H-abstraction reaction of ^{1}•CH_2-CH_2• + SiH_4

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	1.5903670000	0.3731480000	0.0000000000
H	1.7929570000	0.9502650000	0.9165690000
H	1.7929570000	0.9502650000	-0.9165690000
H	0.0549590000	0.3894520000	0.0000000000
H	-2.0510890000	-0.4298050000	1.2150750000
H	-2.0510890000	-0.4298050000	-1.2150750000
H	-2.1578370000	1.6713160000	0.0000000000
Si	-1.5859910000	0.2959040000	0.0000000000
C	1.9339630000	-1.0615250000	0.0000000000
H	2.9775910000	-1.3963540000	0.0000000000
H	1.1587790000	-1.8354010000	0.0000000000

(4/4)CASPT2/aug-cc-pVTZ energy: -369.68217315

Transition state of the H-abstraction reaction of ^{3}•CH_2-CH_2• + SiH_4

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	-1.4492064348	0.7143730047	-0.0003466990
H	-1.5109643175	1.3302911534	-0.9116860082
H	-1.5180733742	1.3190833368	0.9183881707
H	0.0578254391	0.3645972607	-0.0001831935
H	2.1372071149	-0.1714111758	-1.4022791146
H	1.8096470715	-1.3892229584	0.6753266282
H	2.4348570847	0.9580196424	0.7289545003
Si	1.6420621892	-0.0714358774	-0.0004179281

C	-2.1430120089	-0.5876927764	-0.0106331903
H	-3.2368608634	-0.6444800027	-0.0071036200
H	-1.5893239006	-1.5315236072	0.0154354545

(4/4)CASPT2/aug-cc-pVTZ energy: -369.55701530

CH_3-CH_2•

(1/1)CASPT2/aug-cc-pVTZ geometry:

C	0.0236838521	-0.7915824240	0.0000000000
H	-0.0438046296	-1.3442806039	-0.9224708440
H	-0.0438046296	-1.3442806039	0.9224708440
C	0.0011428273	0.6945420549	0.0000000000
H	-1.0229223905	1.0819558694	0.0000000000
H	0.4917809951	1.1025267788	0.8817856233
H	0.4917809951	1.1025267788	-0.8817856233

(1/1)CASPT2/aug-cc-pVTZ energy: -78.96092550

^{1}•CH_2-CH_2-CH_2-CH_2•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	-1.9013295001	0.1300376263	-0.0184984371
H	-1.9963854501	1.2023761141	-0.0831963865
H	-2.8042164349	-0.4590640748	0.0110611253
C	-0.5649123318	-0.5093504068	0.0237105614
H	-0.4556328670	-1.1194170282	0.9283771573
H	-0.4448039444	-1.2120259041	-0.8097772635
C	0.5649156385	0.5093526833	-0.0237152226
H	0.4448042017	1.2120366547	0.8097641479
H	0.4556386692	1.1194098017	-0.9283893016
C	1.9013330685	-0.1300338867	0.0185098117
H	1.9963895791	-1.2023786452	0.0831067615
H	2.8042193713	0.4590740656	-0.0109459538

(2/2)CASPT2/aug-cc-pVTZ energy: -156.73662227

^{3}•CH_2-CH_2-CH_2-CH_2•

(2/2)CASPT2/aug-cc-pVTZ geometry:

C	0.1437091040	-0.0175703303	-1.9129095860
H	1.1226549454	0.4082784773	-2.0719080229
H	-0.3925024321	-0.3866927237	-2.7718548607
C	-0.4996879302	0.0699709091	-0.5762835223
H	-1.0162789701	1.0309333754	-0.4646292719
H	-1.2729294579	-0.6946843362	-0.4794209241
C	0.4996871422	-0.0699706323	0.5762831190

H	1.2729290045	0.6946835816	0.4794193159
H	1.0162754769	-1.0309347521	0.4646292340
C	-0.1437090811	0.0175714108	1.9129096211
H	-1.1226317834	-0.4083257071	2.0719216236
H	0.3924923339	0.3867259113	2.7718472932

(2/2)CASPT2/aug-cc-pVTZ energy: -156.73505831

Transition state of the addition reaction of ^{1}•CH_2-CH_2-CH_2-CH_2• + ethylene

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	1.8575481475	-0.6626430118	-0.3084611823
H	1.2938410848	-1.3624423048	0.3143983072
H	1.4872607612	-0.5129414348	-1.3272630034
C	3.1587139933	-0.3561524301	0.0093539650
H	3.5813661292	-0.6189529622	0.9834182252
H	3.7813517438	0.2425149791	-0.6619455037
C	0.4874923276	1.0655243046	0.3438378757
H	0.5815393086	0.9562410906	1.4318423122
C	-0.8634464960	0.8144261219	-0.2645336438
H	-1.4905956864	1.7284662278	-0.1825685224
H	-0.7658863439	0.6224858251	-1.3509749923
C	-1.6268740011	-0.3429197213	0.3927747683
H	-1.0262035929	-1.2707703401	0.3462351952
H	-1.7320034418	-0.1165860693	1.4767186146
C	-2.9694674650	-0.5761346379	-0.2232714431
H	-3.4916400123	0.2389929714	-0.7329956396
H	-3.5322024171	-1.4886674109	-0.0106247420
H	1.0946095402	1.8701832027	-0.0857418509

(4/4)CASPT2/aug-cc-pVTZ energy: -234.87985244

Transition state of the addition reaction of ^{3}•CH_2-CH_2-CH_2-CH_2• + ethylene

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	1.8379519998	-0.7029258157	-0.1824619857
H	1.3293378886	-1.3085301760	0.5728458301
H	1.3863915464	-0.6881849530	-1.1792519169
C	3.1545464652	-0.3529786678	-0.0115718235
H	3.6550348162	-0.4809667253	0.9525715963
H	3.7163570417	0.1477791257	-0.8055063421
C	0.4847776909	1.0947788297	0.3500748266
H	0.5443019181	1.0339433197	1.4444613901
C	-0.8532573266	0.8285754983	-0.2860290707
H	-1.4998259873	1.7257778202	-0.1711241283
H	-0.7371501897	0.6873872363	-1.3771858453
C	-1.5970941471	-0.3765838307	0.3093745118
H	-1.0157786459	-1.3008497182	0.1407973575

H	-1.6390249531	-0.2473968960	1.4136552250
C	-2.9801545163	-0.5401080788	-0.2401311320
H	-3.5876601167	0.3427490841	-0.4621465309
H	-3.4806780494	-1.5113819540	-0.2239586545
H	1.1073281449	1.8795403015	-0.0942145681

(4/4)CASPT2/aug-cc-pVTZ energy: -234.87926825

Transition state of the H-abstraction reaction of ^{1}•CH_2-CH_2-CH_2-CH_2• + SiH_4

(4/4)CASPT2/aug-cc-pVTZ geometry:

H	-2.1915130137	-1.3179312493	1.2894130483
H	-2.4801020355	-1.4174175740	-1.1188469158
H	-3.7653654009	0.1745850635	0.1935786977
H	-1.2410542732	0.5941799648	-0.1263914170
C	-0.0489952438	1.5826490869	-0.2164534232
H	0.0060128594	1.7642605879	-1.2993756580
H	-0.4659605662	2.4259575971	0.3507317569
C	1.1089418737	0.8441569494	0.4065746316
H	0.8094708397	0.4421389414	1.3941594138
H	1.9451024643	1.5450298799	0.6088659057
C	1.6282941156	-0.3004900888	-0.4703571379
H	1.9322030583	0.1038059428	-1.4559810668
H	0.7915339106	-0.9990659750	-0.6897609126
C	2.7705950060	-1.0391863765	0.1546937778
H	2.9035887855	-1.0342627154	1.2403772474
H	3.3644996365	-1.7467673614	-0.4293195559
Si	-2.4471145761	-0.5090093633	0.0627995577

(4/4)CASPT2/aug-cc-pVTZ energy: -448.12602876

Transition state of the H-abstraction reaction of ^{3}•CH_2-CH_2-CH_2-CH_2• + SiH_4

(4/4)CASPT2/aug-cc-pVTZ geometry:

H	-2.1221393821	-1.3619236199	1.2450869099
H	-2.4378022765	-1.4107763240	-1.1610554753
H	-3.7275225045	0.1333943123	0.2017481119
H	-1.2214833758	0.5984763416	-0.1316796566
C	-0.0442706143	1.6182313037	-0.2095789435
H	0.0059314729	1.8152879529	-1.2899657894
H	-0.4712016517	2.4464696884	0.3716295643
C	1.1227544053	0.8817980470	0.3995064885
H	0.8569750233	0.5357076181	1.4170421315
H	1.9805292863	1.5727229558	0.5297304781
C	1.5816586871	-0.3183327191	-0.4418116480
H	1.8420097874	0.0249303484	-1.4608573860
H	0.7200096280	-1.0090130385	-0.5745151521
C	2.7370966081	-1.0524490389	0.1629588536

H	2.8082455764	-1.1590627551	1.2495859244
H	3.3914282731	-1.6738223675	-0.4534289374
Si	-2.4020815030	-0.5290053950	0.0403124759

(4/4)CASPT2/aug-cc-pVTZ energy: -448.12587089

CH_3-CH_2-CH_2-CH_2•

(1/1)CASPT2/aug-cc-pVTZ geometry:

C	0.5025800181	0.5239795574	-0.0598454761
H	0.3923744885	1.2497907420	0.7484952764
H	0.4064701642	1.0816402766	-0.9927909831
C	-0.6315489542	-0.4925365474	0.0315773179
H	-0.5089043140	-1.0657653632	0.9606026247
H	-0.5320595595	-1.2248674522	-0.7739701863
C	-1.9811505739	0.1289550863	-0.0095959801
H	-2.1268892626	1.1382775369	0.3434925544
H	-2.8547983841	-0.4476211490	-0.2679387485
C	1.8742438649	-0.1316212411	0.0164925062
H	2.6746693940	0.6034051502	-0.0478661038
H	1.9925767372	-0.6744438983	0.9541330116
H	2.0086323813	-0.8441236982	-0.7971508133

(1/1)CASPT2/aug-cc-pVTZ energy: -157.40452597

Table 7

^{3}CBD

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	1.0172108136	0.0000000000
C	1.0172108136	0.0000000000	0.0000000000
C	0.0000000000	-1.0172108136	0.0000000000
C	-1.0172108136	0.0000000000	0.0000000000
H	0.0000000000	-2.0935598636	0.0000000000
H	0.0000000000	2.0935598636	0.0000000000
H	-2.0935598636	0.0000000000	0.0000000000
H	2.0935598636	0.0000000000	0.0000000000

(4/4)CASPT2/aug-cc-pVTZ energy: -154.31464223

^{1}CBD (rectangular geometry)

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.6739108848	0.7790672581
C	0.0000000000	-0.6739108848	0.7790672581
C	0.0000000000	-0.6739108848	-0.7790672581

C	0.0000000000	0.6739108848	-0.7790672581
H	0.0000000000	-1.4366224071	-1.5395599813
H	0.0000000000	1.4366224071	1.5395599813
H	0.0000000000	1.4366224071	-1.5395599813
H	0.0000000000	-1.4366224071	1.5395599813

(4/4)CASPT2/aug-cc-pVTZ energy: -154.33196356

Transition state of the H-abstraction reaction of ^{3}CBD + SiH_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	0.4337042023	1.0605231904	0.0000000000
C	1.3598285047	0.4739174617	1.0147786548
C	2.1425795842	-0.1176249732	0.0000000000
C	1.3598285047	0.4739174617	-1.0147786548
H	3.0120164024	-0.7664281253	0.0000000000
H	0.0096864096	2.0621549804	0.0000000000
H	1.3924743839	0.4883933575	-2.0890462429
H	1.3924743839	0.4883933575	2.0890462429
Si	-2.1103796871	-0.7684405900	0.0000000000
H	-0.7549645592	0.2885151222	0.0000000000
H	-2.9268036033	-0.5088747360	1.2135605494
H	-2.9268036033	-0.5088747360	-1.2135605494
H	-1.5995829226	-2.1796487709	0.0000000000

(6/6)CASPT2/aug-cc-pVTZ energy: -445.69218547

Transition state of the H-abstraction reaction of ^{1}CBD + SiH_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	1.1146093542	0.1096898073	0.0000000000
C	1.0683267090	-0.9774517202	1.0174132559
C	0.9575388276	-1.9534974559	0.0000000000
C	1.0683267090	-0.9774517202	-1.0174132559
H	0.8292385391	-3.0243799845	0.0000000000
H	1.7963944849	0.9520203228	0.0000000000
H	1.0836774275	-0.9958364365	-2.0940476859
H	1.0836774275	-0.9958364365	2.0940476859
Si	-1.6783889774	1.5037824826	0.0000000000
H	-0.1227751811	0.7753807174	0.0000000000
H	-1.8470678542	2.3432530453	1.2086313017
H	-1.8470678542	2.3432530453	-1.2086313017
H	-2.6923426119	0.4248043330	0.0000000000

(6/6)CASPT2/aug-cc-pVTZ energy: -445.69623605

•CBD-H

(5/5)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.0000000000	-1.0535537541
C	0.0000000000	1.0161328563	0.0865621271
C	0.0000000000	0.0000000000	1.0457878419
C	0.0000000000	-1.0161328563	0.0865621271
H	0.0000000000	0.0000000000	2.1254785882
H	0.8895914964	0.0000000000	-1.6842752769
H	0.0000000000	-2.0929150337	0.1193498119
H	0.0000000000	2.0929150337	0.1193498119
H	-0.8895914964	0.0000000000	-1.6842752769

(5/5)CASPT2/aug-cc-pVTZ energy: -154.96177449

Transition state of the addition reaction of ^{3}CBD + C_2H_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.2850906263	-0.1599919401	0.7411473369
C	-0.9107920328	1.0509077178	0.1857251566
C	-1.8994915063	0.2624717042	-0.4548485115
C	-1.3718836306	-0.9257645271	0.1014421501
H	-2.7207468326	0.4806698743	-1.1189129654
H	0.1776147921	-0.3071707697	1.7046206145
H	-1.6302777614	-1.9705096356	0.0520795204
H	-0.6798883180	2.1022469896	0.2252308237
C	1.4748555928	-0.5312459867	-0.4303885168
C	2.4754921164	0.3301095858	-0.0600025407
H	1.5155242071	-1.5628863179	-0.1084270747
H	0.9072109405	-0.3430504270	-1.3305704640
H	2.5468146445	1.3183942491	-0.4887157109
H	3.1563694148	0.0872934831	0.7418941818

(6/6)CASPT2/aug-cc-pVTZ energy: -232.69860281

Transition state of the addition reaction of ^{1}CBD + C_2H_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.2863490000	-0.2343800000	0.6922530000
C	-0.9031180000	1.0480310000	0.2109550000
C	-1.9193910000	0.3345260000	-0.4216090000
C	-1.3990730000	-0.9168480000	0.0506840000
H	-2.7625740000	0.6126120000	-1.0357020000
H	0.1443460000	-0.4391240000	1.6614530000
H	-1.7078330000	-1.9471650000	-0.0254730000
H	-0.6348350000	2.0886120000	0.2945450000
C	1.5080770000	-0.5585460000	-0.4260310000
C	2.4576200000	0.3581460000	-0.0568430000
H	1.5972160000	-1.5813470000	-0.0822550000

H	0.9877860000	-0.4335940000	-1.3658950000
H	2.5123030000	1.3311290000	-0.5259490000
H	3.1169910000	0.1833060000	0.7828190000

(6/6)CASPT2/aug-cc-pVTZ energy: -232.70456751

Transition state of the addition reaction of ^{1}CBD + C_2H_4 (concerted)

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	0.5666386616	-0.5754618990	-0.7871931970
C	0.5666386616	-0.5754618990	0.7871931970
C	-0.5666315962	-1.3416380863	0.7410108903
C	-0.5666315962	-1.3416380863	-0.7410108903
H	-1.2181675169	-1.7575012687	1.4933401689
H	1.3284361010	-0.4113253986	-1.5307334783
H	-1.2181675169	-1.7575012687	-1.4933401689
H	1.3284361010	-0.4113253986	1.5307334783
C	-0.0053617333	1.6840155816	-0.6834800282
C	-0.0053617333	1.6840155816	0.6834800282
H	0.8744010900	1.9786420243	-1.2356162075
H	-0.9207860063	1.5941470468	-1.2456540580
H	-0.9207860063	1.5941470468	1.2456540580
H	0.8744010900	1.9786420243	1.2356162075

(6/6)CASPT2/aug-cc-pVTZ energy: -232.72172856

Product of the addition reaction of ^{3}CBD + C_2H_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.0305577246	-0.2295475748	0.4919269298
C	-0.7694366404	1.0512178595	0.1052959059
C	-1.9122484044	0.3312223050	-0.2527530860
C	-1.3376892374	-0.9016217116	0.0670620743
H	-2.8813802356	0.6204727631	-0.6317118499
H	0.1857744222	-0.3090539264	1.5592534364
H	-1.6657336691	-1.9281000825	0.0338195595
H	-0.4981742595	2.0943193711	0.1182998569
C	1.2158391316	-0.5718946928	-0.3336930428
C	2.3518205100	0.3413909253	-0.0392867448
H	1.4966292787	-1.6059235108	-0.1238490182
H	0.9396723338	-0.5139454951	-1.3881587388
H	2.4311225527	1.2962339280	-0.5340967350
H	3.0314969419	0.1359938421	0.7724764526

(6/6)CASPT2/aug-cc-pVTZ energy: -232.73972762

Product of the addition reaction of ^{1}CBD + C_2H_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.0305538794	-0.2287178337	0.4919801301
C	-0.7698298225	1.0514860829	0.1050427330
C	-1.9124255806	0.3309651303	-0.2527813749
C	-1.3374747192	-0.9014507103	0.0679471653
H	-2.8817498277	0.6197514019	-0.6315614961
H	0.1860438237	-0.3083656370	1.5593070436
H	-1.6644607756	-1.9282540252	0.0332714513
H	-0.4987167695	2.0946631394	0.1169853826
C	1.2153126832	-0.5716914178	-0.3335831061
C	2.3523574017	0.3408192727	-0.0393076487
H	1.4956663343	-1.6058867981	-0.1239717112
H	0.9394942576	-0.5134499790	-1.3881817810
H	2.4307445280	1.2967520239	-0.5321808575
H	3.0327273460	0.1341433499	0.7716190695

(6/6)CASPT2/aug-cc-pVTZ energy: -232.73972787

Product of the addition reaction of ^{1}CBD + C_2H_4 (concerted)

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.5753301902	-0.0870285884	0.7883984624
C	-0.5753301902	-0.0870285884	-0.7883984624
C	0.2608817500	-1.3359743292	-0.6735459536
C	0.2608817500	-1.3359743292	0.6735459536
H	0.7727511799	-1.9343439886	-1.4155690772
H	-1.4853003809	-0.1077659665	1.3810229316
H	0.7727511799	-1.9343439886	1.4155690772
H	-1.4853003809	-0.1077659665	-1.3810229316
C	0.2625021134	1.2259197074	0.7746563941
C	0.2625021134	1.2259197074	-0.7746563941
H	-0.2768333718	2.0753459726	1.1871020169
H	1.2313198997	1.1568231926	1.2637315319
H	1.2313198997	1.1568231926	-1.2637315319
H	-0.2768333718	2.0753459726	-1.1871020169

(6/6)CASPT2/aug-cc-pVTZ energy: -232.83004136

^{3}TMM

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.0000000000	1.4575009495
C	0.0000000000	0.0000000000	-0.0419275748
C	0.0000000000	1.2075240271	-0.7156730378
C	0.0000000000	-1.2075240271	-0.7156730378
H	0.0000000000	-0.9292942543	2.0013663702
H	0.0000000000	0.9292942543	2.0013663702

H	0.0000000000	2.1468767193	-0.1853537064
H	0.0000000000	-2.1468767193	-0.1853537064
H	0.0000000000	-1.2319088613	-1.7947958133
H	0.0000000000	1.2319088613	-1.7947958133

(4/4)CASPT2/aug-cc-pVTZ energy: -155.55851828

$^1B_1$ TMM

(4/4)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	1.2105188625	-0.7125350996
C	0.0000000000	0.0000000000	-0.0314044957
C	0.0000000000	-1.2105188625	-0.7125350996
C	0.0000000000	0.0000000000	1.4522575211
H	0.0000000000	2.1506266612	-0.1852817301
H	0.0000000000	1.2287799894	-1.7925209711
H	0.0000000000	-1.2287799894	-1.7925209711
H	-0.9273431019	0.0000000000	2.0015602881
H	0.9273431019	0.0000000000	2.0015602881
H	0.0000000000	-2.1506266612	-0.1852817301

(4/4)CASPT2/aug-cc-pVTZ energy: -155.53308778

Transition state of the H-abstraction reaction of ^{3}TMM + SiH_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	1.1654469220	0.5210760318	0.0000000000
C	0.0155094943	1.4336966261	0.0000000000
C	-0.5545093638	1.8308977781	1.2250689698
C	-0.5545093638	1.8308977781	-1.2250689698
H	1.7631366076	0.4787033372	-0.9191925748
H	1.7631366076	0.4787033372	0.9191925748
H	-0.1213358829	1.5175344180	2.1781363864
H	-0.1213358829	1.5175344180	-2.1781363864
H	-1.4377313937	2.4745547561	-1.2485617970
H	-1.4377313937	2.4745547561	1.2485617970
Si	-0.0491980620	-2.3783694501	0.0000000000
H	0.6274783784	-0.8135221806	0.0000000000
H	-0.8915855048	-2.5453598686	1.2179154563
H	-0.8915855048	-2.5453598686	-1.2179154563
H	1.0299799324	-3.4071590687	0.0000000000

(6/6)CASPT2/aug-cc-pVTZ energy: -446.93856995

Transition state of the H-abstraction reaction of $^1B_1$ TMM + SiH_4

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.5425894743	-1.0510230012	0.0000000000
C	-1.4728396344	0.1343843561	0.0000000000
C	-2.8549362773	-0.1132572247	0.0000000000
C	-0.9821391934	1.4448535088	0.0000000000
H	-0.5345516995	-1.6562617091	0.9168850438
H	-0.5345516995	-1.6562617091	-0.9168850438
H	-3.2512709413	-1.1312108330	0.0000000000
H	0.0860271523	1.6658104941	0.0000000000
H	-1.6770791062	2.2895421397	0.0000000000
H	-3.5675170920	0.7171380159	0.0000000000
Si	2.5461192896	-0.1693844240	0.0000000000
H	0.9633154697	-0.5663289633	0.0000000000
H	2.8622352677	0.6335874948	-1.2148230127
H	2.8622352677	0.6335874948	1.2148230127
H	3.3691418809	-1.4114601598	0.0000000000

(6/6)CASPT2/aug-cc-pVTZ energy: -446.92293462

- TMM-H

(3/3)CASPT2/aug-cc-pVTZ geometry:

C	0.0147337882	1.4212817389	0.0000000000
C	-0.0081476094	-0.0868479205	0.0000000000
C	-0.0075956034	-0.7686820964	1.2078816678
C	-0.0075956034	-0.7686820964	-1.2078816678
H	-0.4801358488	1.8210966653	-0.8821885370
H	-0.4801358488	1.8210966653	0.8821885370
H	-0.0188592993	-0.2413754889	2.1491120238
H	-0.0188592993	-0.2413754889	-2.1491120238
H	0.0031561465	-1.8479740530	-1.2318663115
H	0.0031561465	-1.8479740530	1.2318663115
H	1.0413400312	1.7865731276	0.0000000000

(3/3)CASPT2/aug-cc-pVTZ energy: -156.20639128

Transition state of the addition reaction of ^{3}TMM + ethylene

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.7621218633	0.5342120107	0.0000000000
C	-0.7756464240	-0.9064589035	0.0000000000
C	-0.7496525727	-1.6010476568	1.2147263524
C	-0.7496525727	-1.6010476568	-1.2147263524
H	-1.0155435513	1.0498493455	-0.9140812068
H	-1.0155435513	1.0498493455	0.9140812068
H	-0.7691770127	-1.0743083702	2.1563618713
H	-0.7691770127	-1.0743083702	-2.1563618713
H	-0.7241719498	-2.6795595784	-1.2347077277
H	-0.7241719498	-2.6795595784	1.2347077277

C	1.3477359365	1.0032293853	0.0000000000
C	1.5143189500	2.3632970938	0.0000000000
H	1.4881953381	0.4436499374	-0.9135704168
H	1.4881953381	0.4436499374	0.9135704168
H	1.5306134489	2.9248725293	0.9218548352
H	1.5306134489	2.9248725293	-0.9218548352

(6/6)CASPT2/aug-cc-pVTZ energy: -233.94553301

Transition state of the addition reaction of $^1B_1$ TMM + ethylene

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	0.0042900247	0.8152809959	0.0000000000
C	1.2921160401	0.0586526881	0.0000000000
C	1.3266015471	-1.3277174559	0.0000000000
C	2.4767869541	0.7904236205	0.0000000000
H	-0.2587539982	1.3368624012	0.9095471552
H	-0.2587539982	1.3368624012	-0.9095471552
H	0.4320218229	-1.9260299983	0.0000000000
H	2.4718482495	1.8688437511	0.0000000000
H	3.4316342389	0.2846402202	0.0000000000
H	2.2771584584	-1.8407116761	0.0000000000
C	-1.8575618169	-0.5698684776	0.0000000000
C	-2.9662928478	0.2141712443	0.0000000000
H	-1.4945633945	-1.0044908424	0.9192791563
H	-1.4945633945	-1.0044908424	-0.9192791563
H	-3.4040199428	0.5656484851	-0.9219603092
H	-3.4040199428	0.5656484851	0.9219603092

(6/6)CASPT2/aug-cc-pVTZ energy: -233.92527031

Transition state of the addition reaction of $^1B_1$ TMM + ethylene (concerted)

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	0.3089156921	1.1596000737	0.7786484265
C	1.0350882724	-0.0068233269	0.1857385277
C	0.7241872641	-1.3395337318	0.5440701187
C	2.0719704164	0.2765746320	-0.6871256941
H	0.3966271066	2.1338876749	0.2920721399
H	0.0929318439	1.1572032096	1.8509579474
H	-0.0106433893	-1.5594503724	1.3198060848
H	2.3028731447	1.3039758947	-0.9805481187
H	2.7060646887	-0.5217919512	-1.0858199367
H	1.3245299488	-2.1642293064	0.1502537923
C	-1.9898991293	0.6740358880	-0.1737429413
C	-1.9255834355	-0.6432461174	-0.5196207092
H	-2.4443387756	0.9927988549	0.7684874936
H	-1.7523369124	1.4569430033	-0.8984444649

H	-1.5475560614	-0.9586332849	-1.4955601244
H	-2.2592606740	-1.4297211399	0.1627084585

(6/6)CASPT2/aug-cc-pVTZ energy: -233.92722462

Product of the addition reaction of ^{3}TMM + ethylene

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.5046000250	0.5165840967	0.0000000000
C	-0.5359553515	-0.9913588587	0.0000000000
C	-0.5238044948	-1.6693124593	1.2103031542
C	-0.5238044948	-1.6693124593	-1.2103031542
H	-1.0235690927	0.9010818344	-0.8779305750
H	-1.0235690927	0.9010818344	0.8779305750
H	-0.5405970902	-1.1364954332	2.1488875807
H	-0.5405970902	-1.1364954332	-2.1488875807
H	-0.5005530483	-2.7484263633	-1.2412546679
H	-0.5005530483	-2.7484263633	1.2412546679
C	0.9491690557	1.0463526476	0.0000000000
C	1.0164705405	2.5300959955	0.0000000000
H	1.4550306059	0.6400082654	-0.8769256031
H	1.4550306059	0.6400082654	0.8769256031
H	0.9620005102	3.0849342154	0.9232674677
H	0.9620005102	3.0849342154	-0.9232674677

(6/6)CASPT2/aug-cc-pVTZ energy: -233.98140741

Product of the addition reaction of $^{1}B_1$ TMM + ethylene

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.0043870301	0.6502737158	0.0000000000
C	1.0381414328	-0.4508471898	0.0000000000
C	0.6898467835	-1.7881385952	0.0000000000
C	2.3784201190	-0.0690090007	0.0000000000
H	0.1645784704	1.2853511849	0.8716089619
H	0.1645784704	1.2853511849	-0.8716089619
H	-0.3349840410	-2.1194457138	0.0000000000
H	2.6633336164	0.9721348764	0.0000000000
H	3.1638711782	-0.8096117857	0.0000000000
H	1.4602523565	-2.5449794064	0.0000000000
C	-1.4680953794	0.1863937670	0.0000000000
C	-2.4124038810	1.3361937058	0.0000000000
H	-1.6406012574	-0.4375237840	0.8780697811
H	-1.6406012574	-0.4375237840	-0.8780697811
H	-2.6999012905	1.8130089124	-0.9235871436
H	-2.6999012905	1.8130089124	0.9235871436

(6/6)CASPT2/aug-cc-pVTZ energy: -233.97918140

Product of the addition reaction of $^1B_1$ TMM + ethylene (concerted)

(6/6)CASPT2/aug-cc-pVTZ geometry:

C	1.2233295988	-0.1358309834	-0.0183259294
C	0.0000000000	0.0000000000	0.8667698249
C	-1.2233295988	0.1358309834	-0.0183259294
C	0.0000000000	0.0000000000	2.2019050415
H	1.5467231337	-1.1793755211	-0.0289268565
H	2.0608530136	0.4628961985	0.3345539174
H	-1.5467231337	1.1793755211	-0.0289268565
H	0.9193232154	-0.0842006549	2.7640306560
H	-0.9193232154	0.0842006549	2.7640306560
H	-2.0608530136	-0.4628961985	0.3345539174
C	0.7201596484	0.2594547582	-1.4114306435
C	-0.7201596484	-0.2594547582	-1.4114306435
H	0.7135208385	1.3466278951	-1.5096640336
H	1.3259139063	-0.1458988459	-2.2194332736
H	-0.7135208385	-1.3466278951	-1.5096640336
H	-1.3259139063	0.1458988459	-2.2194332736

(6/6)CASPT2/aug-cc-pVTZ energy: -234.10000567

allyl•

(3/3) CASPT2/aug-cc-pVTZ geometry

C	0.000000000	2.314194525	-0.368963358
C	0.000000000	-2.314194525	-0.368963358
C	0.000000000	0.000000000	0.832284521
H	0.000000000	4.061932304	0.684874545
H	0.000000000	-4.061932304	0.684874545
H	0.000000000	2.443731472	-2.410079229
H	0.000000000	-2.443731472	-2.410079229
H	0.000000000	0.000000000	2.884266318

(3/3) CASPT2/aug-cc-pVTZ energy -116.98153617

Transition state of the addition reaction of allyl• + ethylene

(5/5) CASPT2/aug-cc-pVTZ geometry

C	0.439546519	1.496200113	-0.634303584
C	2.717250432	0.708513129	0.589142908
H	-0.409108700	3.259422308	-0.053027605
H	0.221247246	1.059121577	-2.619768910
H	3.074709138	1.482354090	2.456502241
C	4.382684969	-0.979664262	-0.345445716
H	4.127774142	-1.817402533	-2.195839088

H	6.043756129	-1.536861350	0.703958889
C	-2.477480091	-0.918890670	0.752859332
C	-4.754794721	-0.243300350	-0.285384551
H	-2.100407918	-0.461777257	2.709712315
H	-1.505189540	-2.577733842	0.060308720
H	-5.349028552	-0.955666630	-2.106904797
H	-5.946988923	1.171397765	0.583857344

(5/5) CASPT2/aug-cc-pVTZ energy -195.16048860

Transition state of the H-abstraction reaction of allyl• + SiH4

(5/5) CASPT2/aug-cc-pVTZ geometry

C	1.398873548	1.955639779	-0.438450478
C	3.251147197	0.379925659	0.798271341
H	1.000334087	3.775604780	0.417085234
H	1.464203270	2.015719842	-2.488774984
H	3.483868860	0.650385153	2.818630460
C	4.608459999	-1.442875821	-0.334833014
H	4.450040478	-1.802449130	-2.343740393
H	5.925156917	-2.600765824	0.712634621
Si	-4.015535748	-0.420679493	0.041175243
H	-1.017912319	0.846102199	-0.138887312
H	-4.396054782	-1.527046113	2.595038064
H	-5.920973063	1.598160287	-0.393178309
H	-4.322058776	-2.422343552	-1.905193540

(5/5) CASPT2/aug-cc-pVTZ energy -408.19386332

Product of the addition reaction of allyl• + ethylene

(3/3) CASPT2/aug-cc-pVTZ geometry

C	0.022903481	-0.848012712	-0.559923963
C	2.533826055	0.456074063	-0.669482725
H	-0.444722479	-1.591704982	-2.435212587
H	0.128025166	-2.468940419	0.712751784
H	2.648507865	2.070191198	-1.935761750
C	4.565306213	-0.191070209	0.649706741
H	4.543859711	-1.782036308	1.939250184
H	6.324628013	0.837352767	0.486345586
C	-2.137212224	0.912006397	0.280206701
C	-4.660701478	-0.314025240	0.253421723
H	-2.141518910	2.580596777	-0.967418837
H	-1.725378539	1.659891970	2.163617368
H	-6.192150653	0.405741208	1.395884001
H	-5.085978674	-1.800931680	-1.083019053

(3/3) CASPT2/aug-cc-pVTZ energy -195.40148363

Product of the H-abstraction reaction of allyl• + SiH4

(2/2) CASPT2/aug-cc-pVTZ geometry

C	2.142673533	-0.955902846	0.000000000
C	0.000000000	0.891058783	0.000000000
H	3.350006330	-0.691722912	1.655800713
H	3.350006330	-0.691722912	-1.655800713
H	1.464978058	-2.901578099	0.000000000
H	0.526458803	2.875675623	0.000000000
C	-2.433334199	0.289730921	0.000000000
H	-3.055356452	-1.661866734	0.000000000
H	-3.892136632	1.721895774	0.000000000

(2/2) CASPT2/aug-cc-pVTZ energy -117.62709807

Table 11

^{3}O2

(6/4)CASPT2/aug-cc-pVTZ geometry:

O	0.0000000000	0.0000000000	0.6027988699
O	0.0000000000	0.0000000000	-0.6027988699

(6/4)CASPT2/aug-cc-pVTZ energy: -150.11222547

$^{1}O_2$

(6/4)CASPT2/aug-cc-pVTZ geometry:

O	0.0000000000	0.0000000000	0.6075910254
O	0.0000000000	0.0000000000	-0.6075910254

(6/4)CASPT2/aug-cc-pVTZ energy: -150.07522750

Reagents of the dimerization reaction of $^{1}O_2$ (MOLCAS)

(8/6)CASPT2/aug-cc-pVTZ geometry:

O	0.08275363	2.49862999	0.60004794
O	-0.08275363	-2.49862999	0.60004794
O	-0.08275363	2.49862999	-0.60004794
O	0.08275363	-2.49862999	-0.60004794

(8/6)CASPT2/aug-cc-pVTZ energy: -300.2207479776

Transition state of the dimerization reaction of $^{1}O_2$ (MOLCAS)

(8/6)CASPT2/aug-cc-pVTZ geometry:

O	0.20969081	0.66848153	0.78480198
O	-0.20969081	-0.66848153	0.78480198
O	-0.20969081	0.66848153	-0.78480198
O	0.20969081	-0.66848153	-0.78480198

(8/6)CASPT2/aug-cc-pVTZ energy: -300.0500356507

Product of the dimerization reaction of $^1O_2$ (MOLCAS)

(8/6)CASPT2/aug-cc-pVTZ geometry:

O	0.72122833	0.71714327	-0.16746048
O	-0.72122833	-0.71714327	-0.16746048
O	-0.72122833	0.71714327	0.16746048
O	0.72122833	-0.71714327	0.16746048

(8/6)CASPT2/aug-cc-pVTZ energy: -300.0600782641

Transition state of the H-abstraction reaction of $^3O_2$ + SiH_4

(8/6)CASPT2/aug-cc-pVTZ geometry:

Si	-0.3972485802	1.5074283477	0.0000000000
H	-1.2192384048	1.5422926043	-1.2246763245
H	0.6362232051	2.5613101341	0.0000000000
H	-1.2192384048	1.5422926043	1.2246763245
H	0.4831330277	-0.1939488984	0.0000000000
O	0.8955577605	-1.2284048195	0.0000000000
O	-0.0867816035	-2.0406689725	0.0000000000

(8/6)CASPT2/aug-cc-pVTZ energy: -441.44060171

Transition state of the H-abstraction reaction of $^1O_2$ + SiH_4

(8/6)CASPT2/aug-cc-pVTZ geometry:

Si	-0.3810571144	1.4462041535	0.0000000000
H	-1.2073714610	1.5296243978	-1.2207252823
H	0.6814373658	2.4722552266	0.0000000000
H	-1.2073714610	1.5296243978	1.2207252823
H	0.4298085691	-0.1467681394	0.0000000000
O	0.9095619063	-1.2553283241	0.0000000000
O	-0.0293690448	-2.1063123122	0.0000000000

(8/6)CASPT2/aug-cc-pVTZ energy: -441.42761885

Transition state of the addition reaction of $^3O_2$ + ethylene

(8/6)CASPT2/aug-cc-pVTZ geometry:

C	0.0028774485	0.8201204806	0.0000000000
C	-1.3623595283	1.2273464706	0.0000000000
H	0.5664955736	1.0107150594	-0.9029698942
H	0.5664955736	1.0107150594	0.9029698942
H	-1.9101813852	1.3195011140	0.9235571172
H	-1.9101813852	1.3195011140	-0.9235571172
O	0.0722548774	-0.8604726189	0.0000000000
O	1.2733138257	-1.2413226792	0.0000000000

(8/6)CASPT2/aug-cc-pVTZ energy: -228.45000475

Transition state of the addition reaction of $^1O_2$ + ethylene

(8/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.0135194318	0.8677017559	0.0000000000
C	-1.3720428345	1.2467690833	0.0000000000
H	0.5534350161	1.0095296573	-0.9086846228
H	0.5534350161	1.0095296573	0.9086846228
H	-1.9204785293	1.3390802974	0.9234244356
H	-1.9204785293	1.3390802974	-0.9234244356
O	0.1087297615	-0.9277577123	0.0000000000
O	1.3096345312	-1.2778290363	0.0000000000

(8/6)CASPT2/aug-cc-pVTZ energy: -228.43866075

Product of the addition reaction of $^3O_2$ + ethylene

(8/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.0152359481	-0.7171590009	0.0000000000
C	1.4063039376	-1.1236905392	0.0000000000
H	-0.5479567710	-1.0388240715	-0.8897252509
H	-0.5479567710	-1.0388240715	0.8897252509
H	1.9486487824	-1.2157950603	0.9254095664
H	1.9486487824	-1.2157950603	-0.9254095664
O	-0.0705875731	0.7590341361	0.0000000000
O	-1.2964794393	1.1622696677	0.0000000000

(8/6)CASPT2/aug-cc-pVTZ energy: -228.45313872

Product of the addition reaction of $^1O_2$ + ethylene

(8/6)CASPT2/aug-cc-pVTZ geometry:

C	-0.0134099985	-0.7047930708	0.0000000000
C	1.4119032025	-1.1213537651	0.0000000000
H	-0.5437098304	-1.0341451718	-0.8886765208

H	-0.5437098304	-1.0341451718	0.8886765208
H	1.9505855894	-1.2278818021	0.9257896553
H	1.9505855894	-1.2278818021	-0.9257896553
O	-0.0773606117	0.7648965662	0.0000000000
O	-1.3094991103	1.1565202174	0.0000000000

(8/6)CASPT2/aug-cc-pVTZ energy: -228.45117328

Table 9

^{1}PQDM

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.0000000000	-2.7934469317
H	0.0000000000	-0.9249422034	-3.3510032124
C	0.0000000000	0.0000000000	-1.4371613995
C	0.0000000000	-1.2354372761	-0.6756534977
C	0.0000000000	1.2354372761	-0.6756534977
C	0.0000000000	-1.2354372761	0.6756534977
H	0.0000000000	-2.1686258630	-1.2228531455
C	0.0000000000	1.2354372761	0.6756534977
H	0.0000000000	2.1686258630	-1.2228531455
C	0.0000000000	0.0000000000	1.4371613995
H	0.0000000000	-2.1686258630	1.2228531455
H	0.0000000000	2.1686258630	1.2228531455
C	0.0000000000	0.0000000000	2.7934469317
H	0.0000000000	-0.9249422034	3.3510032124
H	0.0000000000	0.9249422034	3.3510032124
H	0.0000000000	0.9249422034	-3.3510032124

(8/8)CASPT2/aug-cc-pVTZ energy: -308.92014258

^{3}PQDM

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	0.0000000000	-2.8559487390
H	0.0000000000	-0.9270432130	-3.4063523238
C	0.0000000000	0.0000000000	-1.4224797877
C	0.0000000000	-1.2055361945	-0.6944521713
C	0.0000000000	1.2055361945	-0.6944521713
C	0.0000000000	-1.2055361945	0.6944521713
H	0.0000000000	-2.1440120325	-1.2319994212
C	0.0000000000	1.2055361945	0.6944521713
H	0.0000000000	2.1440120325	-1.2319994212
C	0.0000000000	0.0000000000	1.4224797877
H	0.0000000000	-2.1440120325	1.2319994212
H	0.0000000000	2.1440120325	1.2319994212
C	0.0000000000	0.0000000000	2.8559487390
H	0.0000000000	-0.9270432130	3.4063523238

H	0.0000000000	0.9270432130	3.4063523238
H	0.0000000000	0.9270432130	-3.4063523238

(8/8)CASPT2/aug-cc-pVTZ energy: -308.86180235

Transition state of the addition reaction of ^{1}PQDM + ethylene

(10/10)CASPT2/aug-cc-pVTZ geometry:

C	0.7785980000	2.7251923000	0.0000000000
C	0.5673295000	4.1169211000	0.0000000000
H	1.1795026000	2.2757847000	-0.9164112000
H	1.1795026000	2.2757847000	0.9164112000
H	0.3710658000	4.6544187000	-0.9332110000
H	0.3710658000	4.6544187000	0.9332110000
C	-0.9370655000	1.8086161000	0.0000000000
H	-1.3739229000	2.2199531000	0.9168582000
H	-1.3739229000	2.2199531000	-0.9168582000
C	-0.6461705000	0.4085801000	0.0000000000
C	-0.4002444000	-0.2987265000	1.2279772000
C	-0.4002444000	-0.2987265000	-1.2279772000
C	-0.0001049000	-1.6173895000	1.2345550000
C	-0.0001049000	-1.6173895000	-1.2345550000
H	-0.5627939000	0.2265437000	2.1764107000
H	-0.5627939000	0.2265437000	-2.1764107000
C	0.2223123000	-2.3450009000	0.0000000000
H	0.1583789000	-2.1410459000	2.1835281000
H	0.1583789000	-2.1410459000	-2.1835281000
C	0.6224512000	-3.6721105000	0.0000000000
H	0.7865607000	-4.2109445000	0.9370010000
H	0.7865607000	-4.2109445000	-0.9370010000

(10/10)CASPT2/aug-cc-pVTZ energy: -387.28567669

Transition state of the addition reaction of ^{3}PQDM + ethylene

(10/10)CASPT2/aug-cc-pVTZ geometry:

C	0.8716118000	2.8545317000	0.0000000000
C	0.6713018000	4.2169290000	0.0000000000
H	1.1299939000	2.3330221000	-0.9267722000
H	1.1299939000	2.3330221000	0.9267722000
H	0.5417329000	4.7714267000	-0.9340954000
H	0.5417329000	4.7714267000	0.9340954000
C	-1.1163647000	1.7587799000	0.0000000000
H	-1.5177227000	2.1798144000	0.9267474000
H	-1.5177227000	2.1798144000	-0.9267474000
C	-0.6947295000	0.3561209000	0.0000000000
C	-0.4547455000	-0.3353358000	1.2136701000
C	-0.4547455000	-0.3353358000	-1.2136701000

C	-0.0052881000	-1.6611602000	1.2169058000
C	-0.0052881000	-1.6611602000	-1.2169058000
H	-0.6341555000	0.1783453000	2.1646876000
H	-0.6341555000	0.1783453000	-2.1646876000
C	0.2344995000	-2.3600632000	0.0000000000
H	0.1679799000	-2.1752147000	2.1683443000
H	0.1679799000	-2.1752147000	-2.1683443000
C	0.6965293000	-3.7187473000	0.0000000000
H	0.8752556000	-4.2476557000	0.9386650000
H	0.8752556000	-4.2476557000	-0.9386650000

(10/10)CASPT2/aug-cc-pVTZ energy: -387.25223931

Transition state of the H-abstraction reaction of ^{1}PQDM + SiH_4

(10/10)CASPT2/aug-cc-pVTZ geometry:

Si	3.7637800000	-0.9027080000	0.0000000000
H	5.0644600000	-0.1745580000	0.0000000000
H	3.6568280000	-1.7494940000	-1.2216960000
H	3.6568280000	-1.7494940000	1.2216960000
H	2.2827700000	0.3955460000	0.0000000000
C	1.4872410000	1.3478570000	0.0000000000
H	1.7797970000	1.8956090000	-0.9078910000
H	1.7797970000	1.8956090000	0.9078910000
C	0.1147630000	0.8587480000	0.0000000000
C	-0.5508960000	0.5337280000	1.2229600000
C	-0.5508960000	0.5337280000	-1.2229600000
C	-1.8137670000	-0.0299970000	1.2303020000
C	-1.8137670000	-0.0299970000	-1.2303020000
H	-0.0501420000	0.7569880000	2.1719090000
H	-0.0501420000	0.7569880000	-2.1719090000
C	-2.5031620000	-0.3412350000	0.0000000000
H	-2.3119250000	-0.2522330000	2.1800060000
H	-2.3119250000	-0.2522330000	-2.1800060000
C	-3.7747560000	-0.9124500000	0.0000000000
H	-4.2867390000	-1.1454660000	0.9371940000
H	-4.2867390000	-1.1454660000	-0.9371940000

(10/10)CASPT2/aug-cc-pVTZ energy: -600.27462775

Transition state of the H-abstraction reaction of ^{3}PQDM + SiH_4

(10/10)CASPT2/aug-cc-pVTZ geometry:

Si	3.3266832000	-0.9160131000	0.0000000000
H	4.7911594000	-0.6404531000	0.0000000000
H	2.9702547000	-1.6964288000	-1.2173266000
H	2.9702547000	-1.6964288000	1.2173266000
H	2.4731131000	0.5024042000	0.0000000000

C	1.4972677000	1.6587567000	0.0000000000
H	1.7991141000	2.1699431000	-0.9225914000
H	1.7991141000	2.1699431000	0.9225914000
C	0.1789911000	0.9932276000	0.0000000000
C	-0.4513871000	0.6272572000	1.2135309000
C	-0.4513871000	0.6272572000	-1.2135309000
C	-1.6722080000	-0.0562089000	1.2175574000
C	-1.6722080000	-0.0562089000	-1.2175574000
H	0.0221080000	0.8950295000	2.1644886000
H	0.0221080000	0.8950295000	-2.1644886000
C	-2.3163668000	-0.4201242000	0.0000000000
H	-2.1438991000	-0.3231690000	2.1691612000
H	-2.1438991000	-0.3231690000	-2.1691612000
C	-3.5650099000	-1.1198138000	0.0000000000
H	-4.0515683000	-1.3940727000	0.9385781000
H	-4.0515683000	-1.3940727000	-0.9385781000

(10/10)CASPT2/aug-cc-pVTZ energy: -600.24932440

•PQDMH

(7/7)CASPT2/aug-cc-pVTZ geometry:

C	0.0141282443	1.3525529026	0.0000000000
C	0.0111051846	0.6308748488	1.2020562373
C	0.0111051846	0.6308748488	-1.2020562373
C	0.0022964386	-0.7517027749	1.2104974962
H	0.0187816719	1.1699552214	2.1403880683
C	0.0022964386	-0.7517027749	-1.2104974962
H	0.0187816719	1.1699552214	-2.1403880683
C	-0.0037445784	-1.4916978478	0.0000000000
H	0.0034815677	-1.2878738282	2.1499056900
H	0.0034815677	-1.2878738282	-2.1499056900
C	-0.0103147271	-2.8954619560	0.0000000000
H	-0.0132034531	-3.4486647296	0.9261751878
H	-0.0132034531	-3.4486647296	-0.9261751878
C	-0.0153949140	2.8531582001	0.0000000000
H	0.4783222332	3.2561556799	-0.8822093475
H	-1.0422113406	3.2220455361	0.0000000000
H	0.4783222332	3.2561556799	0.8822093475

(7/7)CASPT2/aug-cc-pVTZ energy: -309.52493539

Product of the addition reaction of ^{1}PQDM + ethylene

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	-0.6065230555	2.6735021293	0.0000000000
C	-0.3868103305	4.1501126132	0.0000000000
H	-1.1869049856	2.3659781115	0.8881329992

H	-1.1869049856	2.3659781115	-0.8881329992
H	-0.1649778825	4.6747498341	0.9340275154
H	-0.1649778825	4.6747498341	-0.9340275154
C	0.7295768223	1.8623477296	0.0000000000
H	1.3185277321	2.1477965646	-0.8889287527
C	0.4700620905	0.3793707905	0.0000000000
C	0.2956369149	-0.3277261383	-1.2136220034
C	0.2956369149	-0.3277261383	1.2136220034
C	-0.0162175781	-1.6865691154	-1.2218941215
H	0.4226778939	0.2036345200	-2.1638796490
C	-0.0162175781	-1.6865691154	1.2218941215
H	0.4226778939	0.2036345200	2.1638796490
C	-0.1854177134	-2.4135024584	0.0000000000
H	-0.1350513090	-2.2163835781	-2.1730607522
H	-0.1350513090	-2.2163835781	2.1730607522
C	-0.4993310163	-3.7929154134	0.0000000000
H	-0.6243210492	-4.3391306188	-0.9378781793
H	-0.6243210492	-4.3391306188	0.9378781793
H	1.3185277321	2.1477965646	0.8889287527

(8/8)CASPT2/aug-cc-pVTZ energy: -387.29872867

Product of the addition reaction of ^{3}PQDM + ethylene

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	-0.5963051275	2.6818184371	0.0000000000
C	-0.3657524204	4.1612946793	0.0000000000
H	-1.1839580952	2.3829156886	0.8871828688
H	-1.1839580952	2.3829156886	-0.8871828688
H	-0.1715330423	4.6933713266	0.9353520740
H	-0.1715330423	4.6933713266	-0.9353520740
C	0.7222111018	1.8634705930	0.0000000000
H	1.3179732752	2.1403655484	-0.8879509039
C	0.4534964999	0.3768554214	0.0000000000
C	0.2897340734	-0.3315488982	-1.2129276149
C	0.2897340734	-0.3315488982	1.2129276149
C	-0.0165732027	-1.6928546917	-1.2210184723
H	0.4157518681	0.1997972908	-2.1632820037
C	-0.0165732027	-1.6928546917	1.2210184723
H	0.4157518681	0.1997972908	2.1632820037
C	-0.1833245549	-2.4191239949	0.0000000000
H	-0.1338039561	-2.2227935076	-2.1723093677
H	-0.1338039561	-2.2227935076	2.1723093677
C	-0.4941537986	-3.8019081595	0.0000000000
H	-0.6155286355	-4.3486489701	-0.9379911207
H	-0.6155286355	-4.3486489701	0.9379911207
H	1.3179732752	2.1403655484	0.8879509039

(8/8)CASPT2/aug-cc-pVTZ energy: -387.29780872

MQDM_symm.out

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	2.4499859238	-1.0438960842
H	0.0000000000	3.3910025722	-0.5164237164
C	0.0000000000	1.2358125723	-0.3466104560
C	0.0000000000	1.2082163000	1.0789124463
C	0.0000000000	0.0000000000	-1.0310655371
C	0.0000000000	0.0000000000	1.7639130594
H	0.0000000000	2.1437918580	1.6200525365
C	0.0000000000	-1.2358125723	-0.3466104560
H	0.0000000000	0.0000000000	-2.1134662459
C	0.0000000000	-1.2082163000	1.0789124463
H	0.0000000000	0.0000000000	2.8446933444
H	0.0000000000	2.4683180120	-2.1226137348
H	0.0000000000	-2.1437918580	1.6200525365
C	0.0000000000	-2.4499859238	-1.0438960842
H	0.0000000000	-2.4683180120	-2.1226137348
H	0.0000000000	-3.3910025722	-0.5164237164

(8/8)CASPT2/aug-cc-pVTZ energy: -308.87819195

^{1}MQDM

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	0.0000000000	2.4736468211	-1.0461552159
H	0.0000000000	3.4089697551	-0.5099706101
C	0.0000000000	1.2260434550	-0.3373927677
C	0.0000000000	1.2058340015	1.0687343089
C	0.0000000000	0.0000000000	-1.0201219519
C	0.0000000000	0.0000000000	1.7598600562
H	0.0000000000	2.1424529160	1.6092330199
C	0.0000000000	-1.2260434550	-0.3373927677
H	0.0000000000	0.0000000000	-2.1028376500
C	0.0000000000	-1.2058340015	1.0687343089
H	0.0000000000	0.0000000000	2.8404466588
H	0.0000000000	2.4961553274	-2.1241279291
H	0.0000000000	-2.1424529160	1.6092330199
C	0.0000000000	-2.4736468211	-1.0461552159
H	0.0000000000	-2.4961553274	-2.1241279291
H	0.0000000000	-3.4089697551	-0.5099706101

(8/8)CASPT2/aug-cc-pVTZ energy: -308.86111541

Transition state of the addition reaction of ^{1}MQDM + ethylene

(10/10)CASPT2/aug-cc-pVTZ geometry:

C	-2.8152307000	-0.9015923000	-0.5245435000
C	-4.0407461000	-0.2784863000	-0.4495110000
H	-2.7138753000	-1.9595757000	-0.2631868000
H	-2.0247543000	-0.4918608000	-1.1608850000
H	-4.8806695000	-0.7404139000	0.0778352000
H	-4.1865533000	0.7358803000	-0.8324451000
C	-1.5528381000	-0.4052590000	1.2967096000
H	-1.5294489000	0.6821039000	1.1785390000
C	-0.3239815000	-1.1603695000	1.0266790000
C	0.7362961000	-0.5641342000	0.3001372000
C	-0.1921422000	-2.5038903000	1.4256092000
C	1.8973819000	-1.2954518000	-0.0004696000
H	0.6476469000	0.4799098000	-0.0188671000
C	0.9743918000	-3.2633299000	1.1302929000
H	-1.0037470000	-2.9774796000	1.9907051000
C	2.0190856000	-2.6306458000	0.4042628000
H	2.7115526000	-0.8188530000	-0.5552962000
H	-2.2419995000	-0.7878274000	2.0554890000
H	2.9249438000	-3.1981114000	0.1669698000
C	1.0993630000	-4.6301951000	1.5514117000
H	0.2994601000	-5.1179787000	2.1129461000
H	1.9984495000	-5.2049126000	1.3183897000

(10/10)CASPT2/aug-cc-pVTZ energy: -387.25182292

Transition state of the addition reaction of ^{3}MQDM + ethylene

(10/10)CASPT2/aug-cc-pVTZ geometry:

C	-2.7821606000	-0.8859298000	-0.5060817000
C	-4.0086056000	-0.2505976000	-0.4028463000
H	-2.7109121000	-1.9615753000	-0.3153455000
H	-2.0153867000	-0.4782333000	-1.1727742000
H	-4.8435874000	-0.7151191000	0.1301506000
H	-4.1411896000	0.7826430000	-0.7373177000
C	-1.5792081000	-0.4486191000	1.2437778000
H	-1.5635769000	0.6410415000	1.1447615000
C	-0.3481411000	-1.1720569000	1.0065398000
C	0.7181565000	-0.5722383000	0.2737437000
C	-0.2058245000	-2.5166368000	1.4158996000
C	1.8897425000	-1.2971353000	-0.0082507000
H	0.6222269000	0.4678441000	-0.0551370000
C	0.9749005000	-3.2700456000	1.1410133000
H	-1.0186880000	-2.9941801000	1.9757874000
C	2.0267657000	-2.6241876000	0.4110688000
H	2.7023158000	-0.8173196000	-0.5628540000
H	-2.2686162000	-0.8393419000	1.9985023000
H	2.9416131000	-3.1830667000	0.1902444000
C	1.1035894000	-4.6118938000	1.5725858000

H	0.2996835000	-5.1015904000	2.1272231000
H	2.0094889000	-5.1842325000	1.3600811000

(10/10)CASPT2/aug-cc-pVTZ energy: -387.26240683

Transition state of the H-abstraction reaction of ^{1}MQDM + SiH_4

(10/10)CASPT2/aug-cc-pVTZ geometry:

Si	-3.2034106000	-0.4930400000	-0.6819251000
H	-4.6500367000	-0.5208155000	-0.3257167000
H	-2.7559326000	-1.8683972000	-1.0367326000
H	-2.9958438000	0.4176112000	-1.8416292000
H	-2.3084722000	0.0516889000	0.5955856000
C	-1.2814838000	0.5067586000	1.6133554000
H	-1.4080405000	-0.2745587000	2.3728509000
C	-0.0240614000	0.4955812000	0.8341518000
C	0.3963041000	1.6540413000	0.1382179000
C	0.7308046000	-0.6821943000	0.7042510000
C	1.5609278000	1.6284643000	-0.6493876000
H	-0.1866387000	2.5768106000	0.2257093000
C	1.9139560000	-0.7310559000	-0.0883141000
H	0.4126225000	-1.5869657000	1.2354048000
C	2.3128921000	0.4544693000	-0.7661777000
H	1.8793628000	2.5332177000	-1.1764507000
H	-1.6882811000	1.4862765000	1.8926721000
H	3.2194526000	0.4392468000	-1.3799481000
C	2.6783165000	-1.9360002000	-0.2021885000
H	2.3698994000	-2.8457696000	0.3178473000
H	3.5839651000	-1.9657565000	-0.8121108000

(10/10)CASPT2/aug-cc-pVTZ energy: -600.24918138

Transition state of the H-abstraction reaction of ^{3}MQDM + SiH_4

(10/10)CASPT2/aug-cc-pVTZ geometry:

Si	-3.4002099000	-0.4579442000	-0.6519261000
H	-4.7834174000	-0.4353449000	-0.0966550000
H	-3.0674568000	-1.8414019000	-1.0941414000
H	-3.3176741000	0.4712075000	-1.8138169000
H	-2.2708564000	0.0344728000	0.5339911000
C	-1.2838579000	0.4223969000	1.4942872000
H	-1.4213495000	-0.3778068000	2.2330756000
C	-0.0024862000	0.4518801000	0.7900256000
C	0.4216930000	1.6304106000	0.1151083000
C	0.7860472000	-0.7097428000	0.6748847000
C	1.6197284000	1.6404656000	-0.6231337000
H	-0.1864342000	2.5380756000	0.1863863000
C	2.0051328000	-0.7231267000	-0.0683642000

H	0.4675291000	-1.6280190000	1.1819253000
C	2.4044693000	0.4883522000	-0.7210573000
H	1.9371553000	2.5585682000	-1.1273309000
H	-1.6949888000	1.3898988000	1.8101892000
H	3.3361855000	0.5004972000	-1.2955492000
C	2.7942909000	-1.8953379000	-0.1614538000
H	2.4875681000	-2.8183688000	0.3360336000
H	3.7252338000	-1.8995195000	-0.7330134000

(10/10)CASPT2/aug-cc-pVTZ energy: -600.25697728

Product of the addition reaction of ^{1}MQDM + ethylene

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	2.6965167670	-0.6617852434	0.1462543105
C	4.0831989783	-1.0511806728	-0.2596307519
H	2.2529325212	-1.4386669344	0.7965340095
H	2.7187035356	0.2616542889	0.7654271501
H	4.7462847075	-1.5676696406	0.4391499435
H	4.5266546843	-0.6332353199	-1.1684897111
C	1.7626759604	-0.4118797837	-1.0527737904
H	2.2040674035	0.3708039728	-1.6964567393
C	0.3819956317	0.0121765829	-0.6046456938
C	0.1156203359	1.3676848716	-0.3002173977
C	-0.6311386834	-0.9345207712	-0.4186314936
C	-1.1522905792	1.7571028202	0.1775812267
H	0.8991091849	2.1186536569	-0.4484573381
C	-1.9273324340	-0.5690334326	0.0636463482
H	-0.4355834507	-1.9876280687	-0.6539582535
C	-2.1615129940	0.8104876767	0.3604615706
H	-1.3470345947	2.8102874829	0.4034681952
H	1.6973588983	-1.3310724439	-1.6609103350
H	-3.1462696688	1.1153921408	0.7291661771
C	-2.9438765154	-1.5407391182	0.2399080145
H	-2.7591187920	-2.5927756775	0.0103031237
H	-3.9320810267	-1.2567626169	0.6091135343

(8/8)CASPT2/aug-cc-pVTZ energy: -387.29827847

Product of the addition reaction of ^{3}MQDM + ethylene

(8/8)CASPT2/aug-cc-pVTZ geometry:

C	2.6965167670	-0.6617852434	0.1462543105
C	4.0831989783	-1.0511806728	-0.2596307519
H	2.2529325212	-1.4386669344	0.7965340095
H	2.7187035356	0.2616542889	0.7654271501
H	4.7462847075	-1.5676696406	0.4391499435
H	4.5266546843	-0.6332353199	-1.1684897111

C	1.7626759604	-0.4118797837	-1.0527737904
H	2.2040674035	0.3708039728	-1.6964567393
C	0.3819956317	0.0121765829	-0.6046456938
C	0.1156203359	1.3676848716	-0.3002173977
C	-0.6311386834	-0.9345207712	-0.4186314936
C	-1.1522905792	1.7571028202	0.1775812267
H	0.8991091849	2.1186536569	-0.4484573381
C	-1.9273324340	-0.5690334326	0.0636463482
H	-0.4355834507	-1.9876280687	-0.6539582535
C	-2.1615129940	0.8104876767	0.3604615706
H	-1.3470345947	2.8102874829	0.4034681952
H	1.6973588983	-1.3310724439	-1.6609103350
H	-3.1462696688	1.1153921408	0.7291661771
C	-2.9438765154	-1.5407391182	0.2399080145
H	-2.7591187920	-2.5927756775	0.0103031237
H	-3.9320810267	-1.2567626169	0.6091135343

(8/8)CASPT2/aug-cc-pVTZ energy: -387.29802387

•MQDMH

(7/7)CASPT2/aug-cc-pVTZ geometry:

C	1.1796774683	-0.2380444992	0.0000200684
C	1.0838969040	1.1628997467	0.0000082736
C	0.0144938436	-0.9857517346	0.0000224604
C	-0.1641402731	1.7896162403	-0.0000037213
H	1.9867445774	1.7585584486	-0.0000166589
C	-1.2686719682	-0.3773845433	0.0000100865
H	0.0737622769	-2.0669549105	0.0000123003
C	-1.3269211952	1.0391016040	0.0000089732
H	-0.2210952777	2.8689179649	-0.0000206577
H	-2.2929389736	1.5248232567	-0.0000141515
C	-2.4386446265	-1.1534284210	-0.0000009722
H	-2.3881219109	-2.2311036483	-0.0000024256
H	-3.4114123220	-0.6869258630	-0.0000116130
C	2.5291787587	-0.8999919459	0.0000582281
H	3.1044420186	-0.6097699413	0.8786556288
H	2.4350255921	-1.9835060868	-0.0001485045
H	3.1046601076	-0.6094456672	-0.8782873147

(7/7)CASPT2/aug-cc-pVTZ energy: -309.52498284

Table 8

benzyl•

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.473416080	2.293305493	0.000309915

C	-2.133487574	2.280891882	-0.000066140
C	-3.462339210	-0.000015118	-0.000328812
C	-2.133453559	-2.280907000	-0.000017008
C	0.473446316	-2.293292265	0.000364717
C	1.874600763	0.000013228	0.000470542
H	1.490929667	4.068141944	0.000684081
H	-3.156127988	4.052043368	-0.000102045
H	-5.505862593	-0.000032125	-0.000886282
H	-3.156073186	-4.052071713	-0.000022677
H	1.490984469	-4.068119268	0.000761560
C	4.521899204	0.000009449	-0.000699199
H	5.575822144	-1.748505008	-0.000907069
H	5.575835372	1.748510677	0.000268341

UCCSD(T)/aug-cc-pVTZ energy: -270.40276123

Transition state of the addition reaction of benzyl• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-5.131847997	-0.746534418	-0.981720284
C	-5.515776096	1.762402054	-1.474545741
H	-6.546376036	-1.783827769	0.071161417
H	-4.010945604	-1.865446930	-2.273996271
H	-6.901255266	2.850780371	-0.437549078
H	-4.329101785	2.785552694	-2.785862609
C	-2.391522119	-1.278042570	2.005607917
H	-3.268175520	-0.035742280	3.368695722
C	0.079992107	-0.620145755	1.079538178
C	1.001573747	1.869778182	1.259920096
C	1.628598105	-2.426083320	-0.114065759
C	3.353929402	2.511869327	0.308331495
H	-0.155913744	3.294125239	2.163589022
C	3.980521013	-1.777948831	-1.061432712
H	0.965638715	-4.356036051	-0.273575652
C	4.859848376	0.695054499	-0.857969679
H	4.024995717	4.436425001	0.477724656
H	5.141211590	-3.203223743	-1.958096423
H	-2.810364798	-3.263817811	2.261204715
H	6.698387496	1.199131386	-1.595282234

UCCSD(T)/aug-cc-pVTZ energy: -348.82755541

Transition state of the H-abstraction reaction of benzyl• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	6.206223443	0.000514006	-1.158549517
H	6.102821409	-2.292509918	-2.776822159
H	8.608949748	-0.000642507	0.298474684

H	6.103290061	2.295554267	-2.773991349
H	3.720575955	-0.000617940	0.895216181
C	1.698601120	-0.001479656	2.717847586
H	2.195589644	1.712458482	3.726517254
C	-0.689993813	-0.000712427	1.371049221
C	-1.859016192	-2.275810408	0.650659163
C	-1.858530532	2.275186799	0.652409050
C	-4.101550413	-2.272450475	-0.700954224
H	-0.992089211	-4.053154527	1.177291821
C	-4.101066643	2.273323529	-0.699210007
H	-0.991238835	4.051948881	1.180406090
C	-5.237636755	0.000820141	-1.383908807
H	-4.973398240	-4.047001578	-1.223100672
H	-4.972540305	4.048456667	-1.220001521
H	2.195408230	-1.716358877	3.725200115
H	-6.989324062	0.001415405	-2.436845310

UCCSD(T)/aug-cc-pVTZ energy: -561.81840026

Product of the addition reaction of benzyl• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-4.730317099	-0.852340185	-0.528847417
C	-5.045313658	1.684242981	-1.685501539
H	-6.542173285	-1.517727873	0.208986703
H	-4.119124866	-2.216688436	-1.954694916
H	-6.379392277	3.024941310	-0.912221826
H	-3.801006479	2.334783092	-3.166916435
C	-2.796730424	-0.951577263	1.696486517
H	-3.374973392	0.409361923	3.134343225
C	-0.105773641	-0.447634547	0.907325546
C	0.938243355	1.969092739	1.064320213
C	1.397186023	-2.392833589	-0.052781941
C	3.401490029	2.433470259	0.277729270
H	-0.190616675	3.502184086	1.814195668
C	3.860054752	-1.939730175	-0.841366545
H	0.631614503	-4.288177876	-0.174145822
C	4.871447515	0.479969650	-0.681348316
H	4.174199044	4.321588234	0.420566109
H	4.993261152	-3.477615757	-1.571515148
H	-2.924169775	-2.825257729	2.554187854
H	6.790645816	0.836649789	-1.288880149

UCCSD(T)/aug-cc-pVTZ energy: -348.86554624

benzylH

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.365565630	2.262255403	-0.016531324
C	2.260777637	2.267803639	0.003616936
C	3.585838482	-0.000051023	0.016247865
C	2.260641576	-2.267875448	0.003616936
C	-0.365656337	-2.262206270	-0.016533214
C	-1.720302735	0.000077479	-0.021771535
H	-1.379728733	4.040559502	-0.034255066
H	3.271824581	4.045461451	0.002825141
H	5.630072402	-0.000109604	0.027503074
H	3.271616711	-4.045574835	0.002823251
H	-1.379898808	-4.040472574	-0.034256955
C	-4.565816439	0.000039684	0.017187059
H	-5.334925526	-1.665498788	-0.921797069
H	-5.283632689	-0.004960531	1.955481042
H	-5.334827260	1.670340266	-0.913312198

UCCSD(T)/aug-cc-pVTZ energy: -271.05619465

^{3}PQDM

UCCSD(T)/aug-cc-pVTZ geometry:

C	-5.401751911	-0.000003779	0.000052912
H	-6.449714655	1.750853937	0.000719986
C	-2.692750133	0.000003779	-0.000077479
C	-1.308058980	2.273442581	-0.000056692
C	-1.308053310	-2.273440692	0.000022677
C	1.308062759	2.273442581	-0.000060471
H	-2.318319797	4.052474225	-0.000117163
C	1.308062759	-2.273444471	0.000009449
H	-2.318316018	-4.052470446	0.000068030
C	2.692718008	0.000001890	-0.000017008
H	2.318295231	4.052481784	-0.000098266
H	2.318297121	-4.052481784	0.000037795
C	5.401776477	0.000000000	0.000054802
H	6.449725993	1.750867166	0.000489439
H	6.449724104	-1.750867166	-0.000298577
H	-6.449720324	-1.750857717	-0.000396842

UCCSD(T)/aug-cc-pVTZ energy: -308.98034042

Transition state of the H-abstraction reaction of ^{3}PQDM + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	6.653652444	-1.220931210	1.067424674
H	9.263252832	-0.525474936	0.295281859
H	6.247106156	-3.958723740	0.598864472
H	6.320224177	-0.673753487	3.800439013
H	4.670076409	0.418871025	-0.568943626

C	2.696382111	2.050504106	-2.197159893
H	3.272987632	1.452151353	-4.069354317
C	0.176761505	1.290301790	-1.339453831
C	-1.013231864	2.519935831	0.688176935
C	-1.105346224	-0.736971818	-2.472599647
C	-3.366495684	1.771667117	1.539448253
H	-0.068437188	4.092575234	1.595123780
C	-3.458776207	-1.496914770	-1.633049015
H	-0.232348763	-1.717436739	-4.042615732
C	-4.670314326	-0.267883362	0.407251439
H	-4.239547248	2.758972505	3.104191549
H	-4.403357742	-3.064583324	-2.547080027
H	3.341623052	3.923503554	-1.676288255
C	-7.081302683	-1.042411163	1.275170696
H	-7.993346516	-0.090817403	2.833438070
H	-8.062966313	-2.601947848	0.397810878

UCCSD(T)/aug-cc-pVTZ energy: -600.40394101

•PQDMH

UCCSD(T)/aug-cc-pVTZ geometry:

C	-2.555032562	0.000005669	-0.023778424
C	-1.185408195	2.268026626	-0.020715178
C	-1.185410084	-2.268022847	-0.020718957
C	1.418915984	2.285534939	-0.004860376
H	-2.201037725	4.045771367	-0.035611889
C	1.418908425	-2.285534939	-0.004860376
H	-2.201043394	-4.045765697	-0.035619448
C	2.831202808	0.000000000	0.006555460
H	2.425493725	4.066694414	-0.007857481
H	2.425486166	-4.066696304	-0.007861261
C	5.474959901	-0.000003779	0.019619137
H	6.528922526	1.748561700	0.025360125
H	6.528916857	-1.748574928	0.025397919
C	-5.394933779	-0.000001890	0.027482287
H	-6.168617893	-1.668571482	-0.902916815
H	-6.108721134	-0.000349599	1.969096519
H	-6.168614114	1.668896515	-0.902329110

UCCSD(T)/aug-cc-pVTZ energy: -309.64731095

Transition state of the addition reaction of ^{3}PQDM + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-5.967785359	-0.233764792	-1.351726771
C	-5.820133497	2.312387947	-1.643543949
H	-7.568400399	-1.068643907	-0.392140849

H	-4.932504567	-1.471864220	-2.604879758
H	-7.047444479	3.578236114	-0.608353864
H	-4.381653179	3.171257136	-2.812891362
C	-3.407941554	-1.503781694	1.859082332
H	-4.303116161	-0.380137309	3.309817525
C	-0.824372238	-0.896166713	1.150612667
C	0.249676286	1.460478620	1.737610737
C	0.681850983	-2.631492771	-0.182360461
C	2.694509468	2.054861739	1.035800467
H	-0.866615176	2.832321526	2.765873086
C	3.126527318	-2.049485468	-0.891782548
H	-0.091869036	-4.467550680	-0.651757094
C	4.217728886	0.319070809	-0.307808041
H	3.471232262	3.884800715	1.519891610
H	4.241350462	-3.428012335	-1.913143618
C	6.726062535	0.918412569	-1.031537244
H	7.547371527	2.730230961	-0.574771541
H	7.875658530	-0.425441603	-2.050522928
H	-4.000735413	-3.458317873	1.766797557

UCCSD(T)/aug-cc-pVTZ energy: -387.41133647

Product of the addition reaction of ^{3}PQDM + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-5.500631831	0.679490715	0.733826010
C	-5.566638075	-1.838637385	1.973015811
H	-7.398495123	1.205811568	0.104303434
H	-4.888984174	2.121157111	2.079949743
H	-6.772591372	-3.322104524	1.250947676
H	-4.264955031	-2.320821795	3.469006164
C	-3.734028916	0.824667035	-1.620731176
H	-4.334642462	-0.600783621	-2.985561307
C	-0.976916600	0.477603713	-1.012277156
C	0.219455785	-1.868954262	-1.292888258
C	0.472809478	2.499981060	-0.094977635
C	2.731754081	-2.197214809	-0.683914564
H	-0.856488133	-3.455464387	-2.009496974
C	2.984134564	2.205956682	0.523737597
H	-0.403059687	4.338569313	0.121713481
C	4.217834710	-0.166692742	0.255507981
H	3.608345121	-4.030088529	-0.925028500
H	4.058470326	3.802350074	1.219109571
C	6.768853494	-0.481574028	0.875283350
H	7.690561745	-2.290718458	0.660995965
H	7.882429419	1.076433358	1.583106728
H	-4.020350771	2.667896455	-2.508545299

UCCSD(T)/aug-cc-pVTZ energy: -387.45677497

^{3}MQDM

UCCSD(T)/aug-cc-pVTZ geometry:

C	-4.631662056	-1.949855327	-0.000462983
H	-6.416549961	-0.958508778	-0.000614161
C	-2.342472387	-0.636140397	-0.000003779
C	-2.280141660	2.063439206	0.000394953
C	0.000100155	-1.924884486	0.000289128
C	0.000032125	3.351136387	0.000037795
H	-4.046120966	3.093606399	0.001262337
C	2.342462939	-0.636282127	0.000005669
H	-0.000224877	-3.971442769	0.000708647
C	2.279822297	2.063227557	-0.000353379
H	0.000141729	5.396583510	0.000013228
H	-4.676100856	-3.991214973	-0.000202201
H	4.045709006	3.093493015	-0.001162182
C	4.631951184	-1.949660685	0.000054802
H	4.676337072	-3.990929624	0.000466762
H	6.416245716	-0.957461870	-0.000241885

UCCSD(T)/aug-cc-pVTZ energy: -308.99716698

Transition state of the addition reaction of ^{3}MQDM + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-5.423253215	-1.583303260	-0.954512007
C	-6.259914342	0.644332360	-1.976812270
H	-6.705216966	-2.685461459	0.198115108
H	-3.996698958	-2.664243614	-1.942254849
H	-7.926269175	1.585351723	-1.257711006
H	-5.185183627	1.631442143	-3.406902205
C	-2.958657277	-0.956656846	2.192084202
H	-4.155851693	0.356836985	3.197643382
C	-0.557951089	-0.056867528	1.292867471
C	-0.121184357	2.558658946	0.947508682
C	1.380452498	-1.735588730	0.649638711
C	2.177614569	3.423751003	0.008934625
H	-1.598897280	3.888733235	1.424435874
C	3.740189423	-0.901057324	-0.305933433
H	1.084952243	-3.745954977	0.903124685
C	4.084969956	1.752925077	-0.612150324
H	2.474768334	5.433089239	-0.232587492
H	-3.048697058	-2.884183170	2.871125162
H	5.868381985	2.442773381	-1.336762030
C	5.660117157	-2.609105185	-0.922074858
H	5.400037929	-4.620639284	-0.686773719
H	7.454381884	-1.960292285	-1.648759593

UCCSD(T)/aug-cc-pVTZ energy: -387.42051784

Transition state of the H-abstraction reaction of ^{3}MQDM + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	-6.683640073	-0.816813333	-1.186319043
H	-9.126840533	-0.793694424	0.201966370
H	-6.227864587	-3.389031065	-2.218256909
H	-6.796502077	1.035658737	-3.294497515
H	-4.282746803	-0.014885373	0.853222687
C	-2.397185628	0.636745110	2.653579890
H	-2.674584196	-0.911403575	3.968559047
C	0.029249181	0.762691577	1.389613890
C	0.857174104	3.031715979	0.250435956
C	1.558213366	-1.376591787	1.164426565
C	3.149154899	3.127744302	-1.036607380
H	-0.303765917	4.708940517	0.397828925
C	3.901156295	-1.328394322	-0.136256813
H	0.950594605	-3.134938489	2.019072216
C	4.658509395	1.008159442	-1.239934353
H	3.755350696	4.887814433	-1.883739479
H	-3.191006663	2.410377806	3.307219151
H	6.438518028	1.099310382	-2.242005097
C	5.410939760	-3.488761361	-0.327234426
H	4.832948125	-5.257873833	0.512410579
H	7.193586449	-3.444721294	-1.321460917

UCCSD(T)/aug-cc-pVTZ energy: -600.41109723

Product of the addition reaction of ^{3}MQDM + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	5.074800944	-1.500062713	0.254820120
C	5.613913354	0.364161564	2.280468583
H	6.846489112	-2.182106448	-0.561791012
H	4.160077121	-3.185817475	1.063919591
H	7.351548657	0.269174480	3.348146840
H	4.173475279	1.664189207	2.916661893
C	3.368019200	-0.508986395	-1.900750794
H	4.280180555	1.119959420	-2.777016801
C	0.732512651	0.206626435	-1.069594439
C	0.056801388	2.743190703	-0.722145613
C	-1.066912918	-1.640701801	-0.613514706
C	-2.373981681	3.391873213	0.078289464
H	1.432280127	4.211855617	-1.087849193
C	-3.553788727	-1.048180062	0.202659900
H	-0.583339560	-3.611688046	-0.893044885

C	-4.154364479	1.548715602	0.539004695
H	-2.860348054	5.362215061	0.332102360
H	3.248817165	-1.976617629	-3.347445751
H	-6.036913430	2.059414089	1.154167242
C	-5.345740429	-2.944971880	0.649908942
H	-4.883517196	-4.916659213	0.389644521
H	-7.236305598	-2.483908939	1.267645296

UCCSD(T)/aug-cc-pVTZ energy: -387.45682737

•MQDMH

UCCSD(T)/aug-cc-pVTZ geometry:

C	2.227342712	-0.448766493	-0.000177634
C	2.042159000	2.198237150	-0.000187083
C	0.027996293	-1.856782536	-0.000153068
C	-0.313855165	3.377983726	0.000022677
H	3.746453865	3.330411760	-0.000479990
C	-2.406044664	-0.714314588	0.000007559
H	0.140162877	-3.901288576	-0.000342040
C	-2.507141233	1.967471354	0.000181414
H	-0.420148480	5.420586811	0.000043464
H	-4.331129461	2.892705835	0.000343930
C	-4.609563599	-2.178141803	-0.000005669
H	-4.521780151	-4.218038801	-0.000162516
H	-6.455087146	-1.304973057	0.000136060
C	4.783240769	-1.703790308	0.000202201
H	5.881014804	-1.158009056	1.660220782
H	4.613802255	-3.755019994	0.000026456
H	5.881906755	-1.157763391	-1.659128521

UCCSD(T)/aug-cc-pVTZ energy: -309.64730224

Table 5 + 6

^{3}TMM

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.000000000	2.664026296	0.000000000
C	0.000000000	0.000000000	0.000000000
C	2.307113722	-1.332013148	0.000000000
C	-2.307113722	-1.332013148	0.000000000
H	-1.748981219	3.716902328	0.000000000
H	1.748981219	3.716902328	0.000000000
H	4.093422701	-0.343788426	0.000000000
H	-4.093422701	-0.343788426	0.000000000
H	-2.344441482	-3.373113901	0.000000000
H	2.344441482	-3.373113901	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -155.62394477

Transition state of the addition reaction of ^{3}TMM + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.373152486	0.975026874	0.000000000
C	-1.462506296	-1.754965982	0.000000000
C	-1.462506296	-3.068225487	2.293753358
C	-1.462506296	-3.068225487	-2.293753358
H	-1.884202462	1.949120224	-1.720219587
H	-1.884202462	1.949120224	1.720219587
H	-1.473648122	-2.080373042	4.081120584
H	-1.473648122	-2.080373042	-4.081120584
H	-1.475089983	-5.109753319	-2.338286644
H	-1.475089983	-5.109753319	2.338286644
C	2.578406584	1.961184235	0.000000000
C	2.862972884	4.531453659	0.000000000
H	2.900803311	0.909160470	-1.722666782
H	2.900803311	0.909160470	1.722666782
H	2.890016754	5.603094671	1.740681542
H	2.890016754	5.603094671	-1.740681542

UCCSD(T)/aug-cc-pVTZ energy: -234.04617774

Product of the addition reaction of ^{3}TMM + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.937451560	0.959960088	0.000000000
C	-1.005404222	-1.902861618	0.000000000
C	-1.005404222	-3.180656633	2.283443012
C	-1.005404222	-3.180656633	-2.283443012
H	-1.925364477	1.687289220	-1.656824945
H	-1.925364477	1.687289220	1.656824945
H	-1.029195874	-2.181826769	4.065243105
H	-1.029195874	-2.181826769	-4.065243105
H	-0.991490168	-5.223136887	-2.350220264
H	-0.991490168	-5.223136887	2.350220264
C	1.812785932	2.015617797	0.000000000
C	1.920878267	4.817960707	0.000000000
H	2.780648854	1.255751360	-1.658726009
H	2.780648854	1.255751360	1.658726009
H	1.825405523	5.873835734	1.746517016
H	1.825405523	5.873835734	-1.746517016

UCCSD(T)/aug-cc-pVTZ energy: -234.08258600

Transition state of the H-abstraction reaction of ^{3}TMM + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	2.084110920	0.951221994	0.000000000
C	0.000000000	2.749806634	0.000000000
C	-1.019928657	3.559839630	2.293502024
C	-1.019928657	3.559839630	-2.293502024
H	3.199553895	0.826539754	-1.715506610
H	3.199553895	0.826539754	1.715506610
H	-0.247282003	2.939531358	4.078941729
H	-0.247282003	2.939531358	-4.078941729
H	-2.607113414	4.846210223	-2.340684706
H	-2.607113414	4.846210223	2.340684706
Si	-0.061412320	-4.584694803	0.000000000
H	1.040555018	-1.550280296	0.000000000
H	-1.612314335	-5.028173842	2.299267579
H	-1.612314335	-5.028173842	-2.299267579
H	2.112332090	-6.365372398	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -447.03668840

- TMMH

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.026567660	2.687432444	0.000000000
C	-0.014027437	-0.174017321	0.000000000
C	-0.014027437	-1.454588344	2.280884323
C	-0.014027437	-1.454588344	-2.280884323
H	-0.907699712	3.451671706	-1.668244560
H	-0.907699712	3.451671706	1.668244560
H	-0.035218826	-0.460329727	4.064838703
H	-0.035218826	-0.460329727	-4.064838703
H	0.005107930	-3.497098833	-2.340327548
H	0.005107930	-3.497098833	2.340327548
H	1.968722353	3.386077423	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -156.27522176

^{3}CBD

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.000000000	1.918720199	0.000000000
C	0.000000000	-1.918720199	0.000000000
C	1.918720199	0.000000000	0.000000000
C	-1.918720199	0.000000000	0.000000000
H	0.000000000	-3.953775719	0.000000000
H	0.000000000	3.953775719	0.000000000
H	-3.953775719	0.000000000	0.000000000

H	3.953775719	0.000000000	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -154.37061072

Transition state of the addition reaction of ^{3}CBD + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.554538244	-0.276259063	1.322405780
C	-1.818517471	1.998453414	0.310852390
C	-3.709513499	0.486621486	-0.801597259
C	-2.638159725	-1.746220329	0.168692072
H	-5.342987098	0.885918728	-1.956960697
H	0.285800290	-0.526583525	3.166058499
H	-3.115068019	-3.725515700	0.092959408
H	-1.422270247	3.995032220	0.382695998
C	2.888130808	-0.988740617	-0.825746069
C	4.791092581	0.589836438	-0.084000216
H	2.905465265	-2.941621395	-0.216296163
H	1.885005596	-0.627236008	-2.569112911
H	5.016249670	2.447085736	-0.907393576
H	6.036849180	0.110760628	1.464426258

UCCSD(T)/aug-cc-pVTZ energy: -232.79011125

Product of the addition reaction of ^{3}CBD + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.068869179	-0.400606822	0.894080455
C	-1.523376265	2.001272886	0.188912142
C	-3.664381170	0.606859091	-0.439786514
C	-2.540190653	-1.704665251	0.121335535
H	-5.525927705	1.128858140	-1.100875076
H	0.351351110	-0.546735564	2.912676460
H	-3.135843668	-3.654095390	0.056897764
H	-1.045562792	3.983083482	0.204842533
C	2.322125706	-1.045587358	-0.650475860
C	4.508234594	0.614249810	-0.055327402
H	2.802966520	-3.020388960	-0.261436051
H	1.838561796	-0.918422018	-2.654347119
H	4.817441032	2.355953693	-1.075531959
H	5.695755503	0.242620048	1.565343303

UCCSD(T)/aug-cc-pVTZ energy: -232.83249506

Transition state of the H-abstraction reaction of ^{3}CBD + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.841336309	1.893611408	0.000000000
C	2.641610365	0.889696291	1.918871378
C	2.641610365	0.889696291	-1.918871378
C	4.195792945	-0.083996437	0.000000000
H	5.925432817	-1.166588412	0.000000000
H	0.000000000	3.764162489	0.000000000
H	2.689788932	0.889148270	-3.955234588
H	2.689788932	0.889148270	3.955234588
Si	-4.083700060	-1.450515984	0.000000000
H	-1.451774542	0.362354986	0.000000000
H	-5.622309407	-0.896550327	2.285746588
H	-5.622309407	-0.896550327	-2.285746588
H	-3.363612358	-4.165355126	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -445.78081232

•CBDH

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.000000000	0.000000000	-1.992094486
C	0.000000000	1.920105369	0.169829687
C	0.000000000	-1.920105369	0.169829687
C	0.000000000	0.000000000	1.969886424
H	0.000000000	0.000000000	4.012825881
H	1.679359929	0.000000000	-3.192350259
H	-1.679359929	0.000000000	-3.192350259
H	0.000000000	-3.957449347	0.234458321
H	0.000000000	3.957449347	0.234458321

UCCSD(T)/aug-cc-pVTZ energy: -155.02216468

allyl•

UCCSD(T)/aug-cc-pVTZ geometry:

C	2.313962089	-0.368851864	0.000064251
H	4.062389618	0.683631105	0.000166296
H	2.442036388	-2.410200172	-0.000343930
C	-2.314084921	-0.368965248	0.000139840
H	-4.062096711	0.684139441	0.000132281
H	-2.442023160	-2.410288989	-0.000719986
C	0.000111494	0.832481053	0.000081258
H	-0.000245664	2.884729301	-0.000946753

UCCSD(T)/aug-cc-pVTZ energy: -117.03570164

Transition state of the addition reaction of allyl• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	3.010498134	-0.720431631	-0.595241055
H	3.966023034	-2.247976632	0.373691453
H	2.478048899	-1.125585135	-2.527006034
C	3.531718616	1.722666782	0.091258654
H	4.427325970	2.156230428	1.876944024
H	2.886928942	3.305639340	-1.027670865
C	-0.578853350	-1.873786292	0.854672107
H	-0.238880280	-3.859310199	0.502618018
H	-0.293449902	-1.291661826	2.793508441
C	-3.712123211	1.497496465	0.122601652
H	-3.264770233	2.447046052	1.879296733
H	-5.148904665	2.348440142	-1.053688614
C	-2.542702099	-0.660525423	-0.552905520
H	-3.063540856	-1.525335911	-2.340008184

UCCSD(T)/aug-cc-pVTZ energy: -195.45573101

Transition state of the addition reaction of allyl• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	1.398913232	1.955709699	-0.438335204
C	3.250948776	0.379757474	0.798352599
C	4.608495904	-1.442769997	-0.334919942
H	1.000398337	3.775542419	0.417493415
H	1.464469722	2.016107236	-2.488621916
H	4.450562042	-1.801714027	-2.343980389
H	5.924856450	-2.601071960	0.712506120
Si	-4.015501733	-0.420675714	0.041097764
H	-1.017931216	0.846302510	-0.138911878
H	-4.321283988	-2.423740059	-1.903931203
H	-4.396171945	-1.525347249	2.595667343
H	-5.921303765	1.597438411	-0.394977328
H	3.483288714	0.649757764	2.818815653

UCCSD(T)/aug-cc-pVTZ energy: -408.44628608

Product of the addition reaction of allyl• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.022882694	0.848649549	0.559147286
C	4.565510303	0.190433371	-0.649500761
H	-0.444524057	1.593647621	2.433997493
H	0.128225477	2.468893176	-0.714407185
H	4.544797015	1.780864678	-1.939703718
H	6.324533527	-0.838337314	-0.485136162
C	-2.137070495	-0.911823094	-0.279900565
C	-4.660879112	0.313660523	-0.253484084

H	-2.141167421	-2.579769077	0.968681174
H	-1.725401216	-1.660765024	-2.162897382
H	-6.192526708	-0.407576132	-1.394744497
H	-5.086383076	1.800846642	1.082618432
C	2.533648421	-0.455677221	0.669571542
H	2.647882366	-2.069270901	1.936574332

UCCSD(T)/aug-cc-pVTZ energy: -195.49404676

allylH

UCCSD(T)/aug-cc-pVTZ geometry:

C	2.325763429	0.306237679	-0.000011338
C	-2.414612682	0.415465739	0.000009449
H	2.228960318	2.363934007	-0.000317474
H	3.407822501	-0.289940680	1.655897089
H	-2.454652200	2.463188092	-0.000039684
H	-4.221020789	-0.541406537	-0.000051023
H	3.408090842	-0.290456576	-1.655558828
C	-0.253542665	-0.854789270	0.000024566
H	-0.314851050	-2.906801302	-0.000068030

UCCSD(T)/aug-cc-pVTZ energy: -117.68527201

•CBDH

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.167546898	1.920018441	-0.001045019
C	-1.970217126	0.002362158	0.000183303
C	-0.171570125	-1.920165840	0.000546131
H	-0.239713649	-3.957434229	-0.003465758
H	-0.229471334	3.957557061	0.000222988
H	-4.013075325	0.004125272	0.001396508
C	1.992190862	-0.001870829	0.000249444
H	3.191486654	-0.002044684	1.680497544
H	3.193629603	-0.004268891	-1.678260108

UCCSD(T)/aug-cc-pVTZ energy: -155.02622508

Transition state of the addition reaction of •CBDH + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.518238494	-0.173975747	1.307767962
C	-1.774403705	2.046390097	0.313772017
C	-3.630141222	0.703773696	-0.834255506
H	-5.240720788	1.199700193	-1.987162300
H	0.297854853	-0.415458180	3.164830177

H	-1.359941410	4.042967013	0.441370104
C	2.955692296	-0.966893493	-0.780585394
C	4.897746834	0.571043112	-0.064906423
H	2.908581424	-2.902770516	-0.120437916
H	1.978923095	-0.618847514	-2.542751232
H	5.188141049	2.398498988	-0.933534158
H	6.118904868	0.092220525	1.502997458
C	-2.611663875	-1.818241571	0.115377229
H	-1.989395957	-3.153652447	-1.330527823
H	-3.816298143	-2.815238402	1.462188822

UCCSD(T)/aug-cc-pVTZ energy: -233.44933317

Transition state of the H-abstraction reaction of •CBDH + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	1.284596140	0.186901473	1.567707350
C	3.958003036	0.118531182	-1.257981237
C	2.811555325	1.955802295	0.099238968
H	5.326138299	0.118007728	-2.773885525
H	0.975293326	0.255969074	3.594274220
H	2.939654191	3.994839468	0.090105921
Si	-4.376813590	0.022688052	-0.264563548
H	-1.341905864	0.178242748	0.716157071
H	-4.513174338	-0.859489019	-2.929037709
H	-5.825492760	-1.750850158	1.364746984
H	-5.530117228	2.578858229	-0.084174071
C	2.617633519	-1.999991651	0.152285470
H	3.826735100	-3.183536576	1.331402766
H	1.387542750	-3.217141576	-0.973180612

UCCSD(T)/aug-cc-pVTZ energy: -446.44125262

Product of the addition reaction of •CBDH + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.032686593	-0.365977591	0.886077465
C	-1.422309932	2.048175888	0.201588425
C	-3.549054963	0.868374511	-0.461280259
H	-5.368216831	1.520702302	-1.128659719
H	0.365223590	-0.547871290	2.904924804
H	-0.861509136	4.013411696	0.260179384
C	2.365438229	-1.038831587	-0.631650408
C	4.562375248	0.603688130	-0.034239948
H	2.825516622	-3.015974560	-0.229000792
H	1.903519242	-0.917533846	-2.642666721
H	4.902206588	2.331665043	-1.068109114
H	5.729241450	0.236253561	1.602283669

C	-2.537467557	-1.753410737	0.083410622
H	-3.482474242	-2.799204075	1.590416189
H	-2.331275760	-2.993547290	-1.552782293

UCCSD(T)/aug-cc-pVTZ energy: -233.49376224

CBDH2

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.317475485	1.485562845	0.000000000
C	1.536989852	1.258489573	0.000000000
C	1.533559999	-1.262962555	0.000001890
H	3.016388410	-2.670337981	0.000001890
H	-2.152910179	2.351412681	-1.675227098
H	3.023644958	2.661958936	-0.000001890
H	-2.152908290	2.351410792	1.675230877
C	-1.321763273	-1.481418675	0.000000000
H	-2.161036002	-2.346234832	-1.674270896
H	-2.161037892	-2.346236722	1.674267117

UCCSD(T)/aug-cc-pVTZ energy: -155.68140366

•TMMH

UCCSD(T)/aug-cc-pVTZ geometry:

C	2.493692467	0.916450315	-0.494751636
C	-0.174136373	0.007585361	0.001509891
C	-1.921781688	1.634679905	1.050908392
H	2.755454137	2.860784278	0.124754239
H	3.869209473	-0.259836342	0.493290405
H	-1.435373174	3.556724001	1.540191369
H	-3.838877271	1.026980567	1.415316490
H	2.940195975	0.822554794	-2.506053090
C	-0.807721011	-2.460964773	-0.619880608
H	0.557402804	-3.740587853	-1.439897896
H	-2.694361465	-3.175927669	-0.297643960

UCCSD(T)/aug-cc-pVTZ energy: -156.27900120

Transition state of the addition reaction of •TMMH + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	3.375158585	-1.285835800	-0.200052077
H	4.238916495	-2.317607371	1.340549041
H	2.360736590	-2.439899108	-1.549055753
C	4.448851840	0.935040269	-0.983449384
H	5.788061065	1.939805764	0.189598112

H	3.850770527	1.861652360	-2.703092604
C	0.032078101	-0.584000964	1.999156392
H	-0.061642866	-2.497885354	2.718274664
C	-1.970674440	0.258869803	0.367710470
H	0.845374654	0.772465240	3.291802765
C	-2.459728004	2.738511741	0.023683938
H	-1.392431472	4.177953930	1.008044169
H	-3.938072095	3.374801427	-1.235852544
C	-3.456583105	-1.737928211	-1.025153750
H	-2.225793137	-2.872638833	-2.235683963
H	-4.362795602	-3.042058450	0.293988474
H	-4.917730688	-0.904536310	-2.209955342

UCCSD(T)/aug-cc-pVTZ energy: -234.70110174

Transition state of the H-abstraction reaction of •TMMH + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.721523893	0.646915616	2.092505084
C	2.670921907	0.218724461	0.217976130
C	3.724328952	2.138899750	-1.079882108
H	0.525355203	-0.753560420	3.578820039
H	0.464734678	2.574139583	2.742829765
H	3.208730405	4.083286210	-0.712245338
H	5.136194367	1.808647432	-2.519932789
Si	-4.621274232	-0.068279585	-0.414065452
H	-1.672417075	0.257471406	0.894380922
H	-5.455280293	2.396836029	-1.470976049
H	-4.563501524	-1.989299581	-2.463601942
H	-6.436286261	-0.888112700	1.568276158
C	3.366407263	-2.490689277	-0.313558478
H	4.048269584	-3.429102707	1.394478045
H	1.716878551	-3.554531390	-0.961063688
H	4.826077081	-2.632962978	-1.756290680

UCCSD(T)/aug-cc-pVTZ energy: -447.69250145

Product of the addition reaction of •TMMH + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.623940325	0.576357021	1.076057302
C	2.071659515	0.251968523	0.205679682
C	3.520495532	2.235124605	-0.337707288
H	-0.923794509	-0.489497650	2.822886123
H	-0.976415823	2.558946185	1.514795018
H	2.822294639	4.150403613	-0.164366489
H	5.454312754	2.012981629	-0.967250651
C	-2.619260574	-0.316427082	-0.897922269

C	-5.261315024	0.041122330	-0.024507858
H	-2.281832965	-2.311926854	-1.313144233
H	-2.290909320	0.728831464	-2.647430721
H	-6.289898626	1.755196528	-0.442917790
H	-6.125617175	-1.288600470	1.264275915
C	3.040472969	-2.413471288	-0.006307906
H	1.953440138	-3.511517443	-1.376062664
H	5.014571593	-2.454535036	-0.585949271
H	2.875184294	-3.398320958	1.803424229

UCCSD(T)/aug-cc-pVTZ energy: -234.73929086

TMMH2

UCCSD(T)/aug-cc-pVTZ geometry:

C	-2.405559004	-1.278008555	-0.000098266
C	0.000083148	0.234441314	0.000069920
C	0.000944863	2.747973600	0.000130391
H	-4.070528669	-0.068513911	-0.002020117
H	-2.498699826	-2.513229930	-1.654850181
H	-1.741101061	3.820209876	0.000323143
H	1.743706993	3.819051474	-0.001046908
H	-2.500343888	-2.510028734	1.656926990
C	2.404614141	-1.279403172	0.000047243
H	2.497991179	-2.512708366	-1.656138974
H	4.070500323	-0.071127402	0.000370386
H	2.497976061	-2.513679685	1.655532372

UCCSD(T)/aug-cc-pVTZ energy: -156.93126686

Fig. XII-6

allyl•

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000	1.224619	-0.195247
C	0.000000	0.000000	0.440426
H	0.000000	2.149482	0.362420
H	0.000000	1.293167	-1.275359
H	0.000000	0.000000	1.526288
C	0.000000	-1.224619	-0.195247
H	0.000000	-1.293167	-1.275359
H	0.000000	-2.149482	0.362420

UB3LYP/aug-cc-pVTZ energy: -117.3092731

^{3}CBD

UB3LYP/aug-cc-pVTZ geometry:

C	0.041350	1.014673	-0.000018
C	1.014687	-0.041350	-0.000164
C	-0.041350	-1.014674	0.000074
C	-1.014687	0.041351	0.000151
H	0.085248	2.091253	-0.000601
H	2.091274	-0.085248	0.000008
H	-0.085249	-2.091253	-0.000361
H	-2.091274	0.085242	0.000695

UB3LYP/aug-cc-pVTZ energy: -154.7254532

^{3}TMM

UB3LYP/aug-cc-pVTZ geometry:

C	0.000000	1.409742	0.000000
C	0.000000	0.000000	0.000000
C	-1.220872	-0.704871	0.000000
C	1.220872	-0.704871	0.000000
H	0.925521	1.966900	0.000000
H	-0.925521	1.966900	0.000000
H	-2.166146	-0.181926	0.000000
H	2.166146	-0.181926	0.000000
H	1.240625	-1.784975	0.000000
H	-1.240625	-1.784975	0.000000

UB3LYP/aug-cc-pVTZ energy: -155.9888142

Fig. XIII-4

Transition state of the H-abstraction reaction of benzyl• + SiH_4 (*ortho* position)

UB3LYP/aug-cc-pVTZ geometry:

14	-2.854350	-0.308417	-0.397577
H	-2.774232	-0.063368	-1.861425
H	-3.762292	0.686547	0.233765
H	-3.364631	-1.682290	-0.141539
H	-1.041473	-0.177117	0.423314
C	0.445707	2.391593	0.400508
H	-0.212439	2.720979	1.193107
C	0.711048	1.084498	0.195577
C	1.624080	0.643875	-0.841720
C	0.041535	0.010290	0.983737
C	2.050456	-0.636757	-0.908758
H	1.998565	1.384506	-1.537113
C	0.712475	-1.295947	1.001976
H	-0.306452	0.345454	1.959160

C	1.632145	-1.613573	0.069588
H	2.753430	-0.933900	-1.675852
H	0.395199	-2.025802	1.735491
H	0.889696	3.156845	-0.221676
H	2.080852	-2.597888	0.053402

UB3LYP/aug-cc-pVTZ energy: -562.8698888

Transition state of the H-abstraction reaction of benzyl• + SiH_4 (*para* position)

UB3LYP/aug-cc-pVTZ geometry:

14	3.172543	0.000334	-0.634214
H	3.957631	-1.222591	-0.314807
H	3.972571	1.206432	-0.288953
H	2.837492	0.017887	-2.082477
H	1.540806	-0.000595	0.403790
C	-3.142613	0.000753	-1.058392
H	-3.612069	-0.922270	-1.369405
C	-2.012483	0.000249	-0.315105
C	-1.375169	1.233605	0.119075
C	-1.375497	-1.233686	0.117919
C	-0.227826	1.236041	0.820015
H	-1.867806	2.167530	-0.122218
C	-0.228165	-1.237087	0.818869
H	-1.868384	-2.167251	-0.124252
C	0.498761	-0.000764	1.126571
H	0.208714	2.174497	1.138882
H	0.208146	-2.175955	1.136830
H	-3.611811	0.924199	-1.368540
H	0.997065	-0.001240	2.096428

UB3LYP/aug-cc-pVTZ energy: -562.8730889

Product of the H-abstraction reaction of benzyl• + SiH_4 (*ortho* position)

UB3LYP/aug-cc-pVTZ geometry:

C	0.276718	1.258363	0.101090
C	-1.066084	1.278557	0.037209
C	-1.835039	0.051070	-0.118457
C	-1.235288	-1.141545	-0.080548
C	1.030481	0.014028	0.025842
H	0.837557	2.183097	0.159215
H	-1.596131	2.221741	0.063432
H	-2.904261	0.124465	-0.269226
H	-1.808523	-2.053667	-0.189328
C	2.357495	0.012712	-0.155222
H	2.920354	-0.906440	-0.251694
H	2.915927	0.937894	-0.209497

C	0.239210	-1.275046	0.179253
H	0.360963	-1.637049	1.210200
H	0.669156	-2.058878	-0.448105

UB3LYP/aug-cc-pVTZ energy: -271.6100994

Product of the H-abstraction reaction of benzyl• + SiH_4 (*para* position)

UB3LYP/aug-cc-pVTZ geometry:

C	0.290603	-1.239353	-0.000064
C	-1.044120	-1.249988	0.000003
C	-1.044120	1.249988	0.000033
C	0.290603	1.239353	-0.000030
C	1.067304	0.000000	-0.000061
H	0.841657	-2.172375	-0.000137
H	-1.576530	-2.193690	-0.000024
H	-1.576530	2.193690	0.000025
H	0.841657	2.172375	-0.000083
C	2.410489	0.000000	-0.000046
H	2.974444	0.922906	0.000043
H	2.974444	-0.922906	0.000054
C	-1.868604	0.000000	0.000117
H	-2.546152	0.000010	-0.865099
H	-2.545925	-0.000010	0.865511

UB3LYP/aug-cc-pVTZ energy: -271.616573

Transition state of the H-abstraction reaction of ^{3}PQDM + SiH_4 (*ortho* position)

UB3LYP/aug-cc-pVTZ geometry:

14	-2.675075	-1.217981	-0.415093
H	-2.847895	-2.508257	0.303136
H	-2.367640	-1.473602	-1.845599
H	-3.921825	-0.416116	-0.301835
H	-1.341832	-0.276708	0.346237
C	-0.729597	2.702806	0.343696
H	-1.476228	2.821947	1.116700
C	-0.045911	1.539489	0.187119
C	0.979343	1.394936	-0.832899
C	-0.333847	0.346748	0.981519
C	1.789050	0.322222	-0.886451
H	1.103690	2.204542	-1.541385
C	0.694786	-0.710968	1.022511
H	-0.838616	0.534195	1.925870
C	1.716107	-0.760624	0.093285
H	2.554883	0.259919	-1.649296
H	0.598340	-1.494649	1.762421
H	-0.543719	3.551361	-0.299914

C	2.670158	-1.792012	0.070515
H	3.448747	-1.815240	-0.677654
H	2.642616	-2.591249	0.796844

UB3LYP/aug-cc-pVTZ energy: -601.5437392

Product of the H-abstraction reaction of ^{3}PQDM + SiH_4 (*ortho* position)

UB3LYP/aug-cc-pVTZ geometry:

C	0.656250	1.251811	0.089115
C	-0.685070	1.236259	0.088459
C	-1.461103	-0.005291	-0.018327
C	-0.751643	-1.208862	-0.026017
C	1.459498	0.041281	0.006343
H	1.185707	2.196548	0.120607
H	-1.237268	2.166610	0.133007
H	-1.295618	-2.141879	-0.102957
C	2.783767	0.096205	-0.179847
H	3.386109	-0.798660	-0.265783
H	3.300815	1.043919	-0.251933
C	0.728501	-1.279794	0.161653
H	0.929002	-1.664656	1.173822
H	1.161142	-2.028419	-0.507987
C	-2.836898	0.049207	-0.117740
H	-3.427312	-0.851711	-0.207429
H	-3.362391	0.993356	-0.113180

UB3LYP/aug-cc-pVTZ energy: -310.2957522

Transition state of the H-abstraction reaction of ^{3}PQDM + SiH_4 (*ortho* 1 position)

UB3LYP/aug-cc-pVTZ geometry:

14	-3.023965	-0.678520	-0.660284
H	-2.682181	-0.712228	-2.106335
H	-4.102337	0.317425	-0.419741
H	-3.484600	-2.022945	-0.220294
H	-1.473574	-0.213967	0.360379
C	-0.387718	2.497284	0.237109
H	-1.282597	2.739636	0.792920
C	0.171773	1.242108	0.285406
C	1.343058	0.926820	-0.433572
C	-0.482210	0.157276	1.062315
C	2.007234	-0.325052	-0.324505
H	1.779519	1.687846	-1.068997
C	0.321806	-1.042508	1.300123
H	-1.026741	0.511455	1.935715
C	1.457444	-1.286696	0.623596
H	-0.055490	-1.772704	2.005200

H	0.057949	3.283678	-0.355844
H	2.005873	-2.205549	0.787930
C	3.136099	-0.611714	-1.047031
H	3.552205	0.102416	-1.743685
H	3.642564	-1.560881	-0.943930

UB3LYP/aug-cc-pVTZ energy: -601.5638392

Transition state of the H-abstraction reaction of ^{3}PQDM + SiH_4 (*ortho* 2 position)

UB3LYP/aug-cc-pVTZ geometry:

14	-2.802463	-0.074239	-0.576504
H	-3.780281	0.466008	0.405305
H	-3.173187	-1.468136	-0.935235
H	-2.792300	0.776948	-1.794491
H	-1.091129	-0.055291	0.208238
C	0.288147	2.435577	1.086736
H	-0.366111	2.437310	1.947457
C	0.618136	1.280918	0.442919
C	1.489919	1.267272	-0.689249
C	0.022343	-0.016044	0.838791
C	1.923883	0.074206	-1.250576
H	1.843249	2.211157	-1.082975
C	0.721660	-1.255089	0.428058
H	-0.346867	-0.036863	1.861054
C	1.588273	-1.156960	-0.703909
H	2.587960	0.106319	-2.104861
H	0.679804	3.388727	0.759375
H	2.017450	-2.064131	-1.108481
C	0.490478	-2.440248	1.059611
H	0.958839	-3.353917	0.720683
H	-0.159974	-2.506576	1.920718

UB3LYP/aug-cc-pVTZ energy: -601.5684912

Product of the H-abstraction reaction of ^{3}PQDM + SiH_4 (*ortho* 1 position)

UB3LYP/aug-cc-pVTZ geometry:

C	0.024349	-1.051587	-0.000238
C	1.275086	-0.366407	-0.000072
C	1.231748	1.099774	-0.000302
C	0.083778	1.775630	-0.000142
C	-1.221519	-0.403007	0.000011
H	0.037325	-2.135142	-0.000583
H	2.177528	1.627503	-0.000624
H	0.094514	2.859139	-0.000341
C	-2.393603	-1.112264	-0.000085
H	-3.355872	-0.618896	0.000107

H	-2.390731	-2.193548	-0.000398
C	-1.261004	1.115633	0.000387
H	-1.832283	1.463077	0.868531
H	-1.833241	1.463522	-0.866941
C	2.461271	-1.032682	0.000317
H	3.403591	-0.502956	0.000474
H	2.498529	-2.113233	0.000515

UB3LYP/aug-cc-pVTZ energy: -

Product of the H-abstraction reaction of ^{3}PQDM + SiH_4 (*ortho* 2 position)

UB3LYP/aug-cc-pVTZ geometry:

C	1.215559	1.111570	0.002242
C	-0.000003	1.781828	0.033516
C	-1.215603	1.111554	0.002577
C	-1.282102	-0.317937	0.016525
C	1.282070	-0.317933	0.016480
H	2.137386	1.671076	-0.090134
H	-0.000062	2.864320	0.009341
H	-2.137405	1.671170	-0.089411
C	2.432397	-0.985320	-0.215256
H	2.471501	-2.066154	-0.223520
H	3.357811	-0.456595	-0.401009
C	0.000003	-1.052042	0.364630
H	0.000045	-1.185981	1.453632
H	-0.000017	-2.053009	-0.065371
C	-2.432345	-0.985374	-0.215459
H	-2.471323	-2.066208	-0.223909
H	-3.357798	-0.456694	-0.401148

UB3LYP/aug-cc-pVTZ energy: -310.3107935

Table 10

O_2

UCCSD(T)/aug-cc-pVTZ geometry:

O	0.000000	0.000000	0.602935
O	0.000000	0.000000	-0.602935

UCCSD(T)/aug-cc-pVTZ energy: -150.128981

O_4

UCCSD(T)/aug-cc-pVTZ geometry:

O	0.000000	1.006305	0.167150

O	-1.006305	0.000000	-0.167150
O	0.000000	-1.006305	0.167150
O	1.006305	0.000000	-0.167150

UCCSD(T)/aug-cc-pVTZ energy: -300.1062916

O_6

UCCSD(T)/aug-cc-pVTZ geometry:

O	0.000000	1.298626	0.295929
O	-1.124643	0.649313	-0.295929
O	-1.124643	-0.649313	0.295929
O	0.000000	-1.298626	-0.295929
O	1.124643	-0.649313	0.295929
O	1.124643	0.649313	-0.295929

UCCSD(T)/aug-cc-pVTZ energy: -450.2541887

O_8

UCCSD(T)/aug-cc-pVTZ geometry:

O	0.000000	1.631665	0.335930
O	1.631665	0.000000	0.335930
O	-1.631665	0.000000	0.335930
O	0.000000	-1.631665	0.335930
O	1.153762	-1.153762	-0.335930
O	-1.153762	1.153762	-0.335930
O	1.153762	1.153762	-0.335930
O	-1.153762	-1.153762	-0.335930

UCCSD(T)/aug-cc-pVTZ energy: -600.3564509

Transition state of the addition reaction of O_2 + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	1.121508995	1.033005562	-0.000124722
C	3.448413819	-0.326841363	-0.000041574
H	0.689366424	2.084058008	1.704311873
H	0.689196348	2.083634709	-1.704801312
H	4.292374958	-0.960761332	-1.747297473
H	4.293382182	-0.958918849	1.747391959
O	-1.279679072	-0.995090097	0.000253223
O	-3.393301846	0.184465616	-0.000079368

UCCSD(T)/aug-cc-pVTZ energy: -228.50895229

Transition state of the H-abstraction reaction of O_2 + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	-0.805437182	2.928489689	0.000000000
H	-2.367804166	3.087551717	-2.320283223
H	-2.367804166	3.087551717	2.320283223
H	1.243810181	4.840323726	0.000000000
H	0.841332530	-0.535385869	0.000000000
O	1.740800594	-2.357045955	0.000000000
O	0.000000000	-4.077826791	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -441.49606286

Product of the addition reaction of O_2 + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-0.957760447	0.996301411	0.000109604
C	-3.402357413	-0.298508699	0.000017008
H	-0.622286815	2.121998039	-1.686658051
H	-0.622158314	2.121491593	1.687198513
H	-4.268583306	-0.888443402	1.750863386
H	-4.269439351	-0.886682178	-1.750995667
O	1.135800994	-0.958661846	-0.000207870
O	3.357096583	0.126770388	0.000062361

UCCSD(T)/aug-cc-pVTZ energy: -228.51445094

Product of the H-abstraction reaction of O_2 + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	1.936986292	-2.663710712	0.000000000
H	1.018843954	-3.920070564	2.327615360
H	1.018843954	-3.920070564	-2.327615360
H	4.718241749	-2.330531208	0.000000000
H	0.000000000	1.479370212	0.000000000
O	-0.898736741	3.142495504	0.000000000
O	-3.335480006	2.605410771	0.000000000

UCCSD(T)/aug-cc-pVTZ energy: -441.50187633

HOO•

UCCSD(T)/aug-cc-pVTZ geometry:

O	0.0553660000	0.7187530000	0.0000000000
O	0.0553660000	-0.6105390000	0.0000000000
H	-0.8858570000	-0.8657060000	0.0000000000

UCCSD(T)/aug-cc-pVTZ energy: -150.71262509

Transition state of the addition reaction of HOO• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	1.750944644	1.035116386	0.686414671
C	3.074835749	-1.009538943	-0.218934221
H	0.984715500	0.997907678	2.578334775
H	2.139202106	2.896060098	-0.062568832
H	4.126925655	-0.899483182	-1.966214686
H	2.947666629	-2.838054955	0.684415341
O	-1.437930408	0.883203192	-0.917131335
O	-3.059702823	-0.651539776	0.480234212
H	-3.172126410	-2.163203518	-0.543672318

UCCSD(T)/aug-cc-pVTZ energy: -229.13045175

Transition state of the H-abstraction reaction of HOO• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	-3.003426778	-0.130595193	-0.000444086
H	-3.352721867	-2.104714604	-1.963433009
H	-4.543791681	2.131790600	-0.608306621
H	-3.671596144	-1.132871919	2.530144869
H	0.085438298	0.711504565	0.018218850
O	2.380346278	1.329915552	-0.035328430
O	3.788615545	-0.885786447	0.227199883
H	4.178972492	-1.330395542	-1.505369064

UCCSD(T)/aug-cc-pVTZ energy: -442.12208991

Product of the addition reaction of HOO• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	-1.187808147	-1.132008314	0.467355728
C	-2.834936907	1.035097488	-0.183416818
H	-0.938997356	-1.324664003	2.506948480
H	-1.962471139	-2.918816181	-0.252157496
H	-3.022473328	1.612153709	-2.135080613
H	-3.929241405	2.009975074	1.235914905
O	1.234864217	-1.062874573	-0.737100906
O	2.694379077	0.930389653	0.453335850
H	2.555720422	2.262701378	-0.789140184

UCCSD(T)/aug-cc-pVTZ energy: -229.15820117

Product of the H-abstraction reaction of HOO• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	-3.243892539	0.044472815	-0.008165507
H	-3.065377670	-1.736586505	-2.165157495
H	-5.461939688	1.743111730	-0.274180364
H	-3.249631637	-1.284862591	2.455918316
H	1.664398967	1.945807534	-0.044814855
O	3.415273691	1.391688809	-0.029929482
O	3.070651896	-1.317416903	0.224643084
H	3.639638985	-1.884270492	-1.415164877

UCCSD(T)/aug-cc-pVTZ energy: -442.14827174

HO•

UCCSD(T)/aug-cc-pVTZ geometry:

O	0.0000000000	0.0000000000	0.1082920000
H	0.0000000000	0.0000000000	-0.8663350000

UCCSD(T)/aug-cc-pVTZ energy: -75.63766551

Product of the addition reaction of HO• + ethylene

UCCSD(T)/aug-cc-pVTZ geometry:

C	0.011943069	1.015366858	-0.057829399
C	-2.331203950	-0.512013736	0.016302667
H	0.113801197	2.135430213	-1.801366317
H	0.036900682	2.376442104	1.507572485
H	-4.033781054	0.205698579	0.885860147
H	-2.423600220	-2.262102335	-1.034356716
O	2.256259302	-0.481439857	-0.080147065
H	2.172179717	-1.624083550	1.332629199

UCCSD(T)/aug-cc-pVTZ energy: -154.12249706

Product of the H-abstraction reaction of HO• + SiH_4

UCCSD(T)/aug-cc-pVTZ geometry:

Si	2.142679202	-0.010142160	0.086524890
H	1.533798104	2.437255381	-1.142670149
H	1.698894028	-2.167338238	-1.645690678
H	4.820387115	0.004008109	0.958947195
H	-3.936779522	-1.047004653	1.394377890
O	-3.759680058	-0.090166393	-0.141676548
H	-4.036362420	1.636397005	0.357112885

UCCSD(T)/aug-cc-pVTZ energy: -367.12211148

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