Supporting Information

Mechanistic Insights into Alkane Metathesis Catalyzed by Silica Supported Tantalum Hydrides: A DFT study

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Text S1. Structures and stabilities of the initial TaH_x/SiO_2 (x= 1, 3) surface species.

According to EXASF and IR spectroscopies, the initial surface Ta-hydride is formed by a mixture of mono (**1a**) and trishydride (**1b**) species.[1-2] Figure 2 shows the optimized geometries around the metal center and the most relevant bond distances. Scheme 3a shows the associated energetics. The computed geometries and IR stretching frequencies are similar to those published before and in reasonable agreement with the experimental measurements (see Tables S1 and S2 of the Supporting Information for further details).[1-3] The trishydride species is found to be 30.3 kcal·mol^{-1} lower in Gibbs energy than **1a** + H_2 at 423 K (Scheme 3a). The tantalum center in the monohydride species is formally a Ta(III) species and thus, shows a d^2 electronic configuration that can lead to two potential spin states (singlet or triplet). The two states are close in energy and the prediction of the most favorable one strongly depends on the functional used. In this view, B3PW91, PBE and PBE0 functionals favor the triplet state, while M06 yields to a more stable singlet by 7.2 kcal mol^{-1}. This shows the difficulties of DFT for properly predict the relative energies of close in energy states of different spin multiplicity,[4-6] but this problem has little influence here since, once **1a** reacts with ethane, the oxidation state of Ta changes from III to V and the entire potential energy surface takes place on the singlet spin state of a Ta(V) metal. The energy barrier for H_2 oxidative addition to **1a** forming **1b** is relatively low (22.2 kcal·mol^{-1}) and it takes place without prior formation of a H_2 adduct. This barrier for the formation of **1b** is attributed to the concerted splitting of H_2 molecule when approaching to the Ta with the concomitant oxidation of tantalum. All these data suggest that **1b** is favored over **1a** both from a thermodynamic and kinetic point of view and thus, the reactivity of the TaH_x/SiO_2 catalyst towards alkanes takes place mainly on **1b**.

References

(1) Vidal, V.; Théolier, A.; Thivolle-Cazat, J.; Basset, J.-M.; Corker, J. Synthesis, Characterization, and Reactivity, in the C−H Bond Activation of Cycloalkanes, of a Silica-Supported Tantalum(III) Monohydride Complex (SiO)2TaIII−H. *J. Am. Chem. Soc.* **1996**, *118*, 4595-4602.

(2) Soignier, S.; Taoufik, M.; Le Roux, E.; Saggio, G.; Dablemont, C.; Baudouin, A.; Lefebvre, F.; de Mallmann, A.; Thivolle-Cazat, J.; Basset, J.-M.; Sunley, G.; Maunders, B. M. Tantalum Hydrides Supported on MCM-41 Mesoporous Silica: Activation of Methane and Thermal Evolution of the Tantalum-Methyl Species. *Organometallics* **2006**, *25*, 1569-1577.

(3) Saggio, G.; Taoufik, M.; Basset, J. M.; Thivolle-Cazat, J. Poisoning Experiments Aimed at Discriminating Active and Less-Active Sites of Silica-Supported Tantalum Hydride for Alkane Metathesis. *ChemCatChem* **2010**, *2*, 1594-1598.

(4) Swart, M.; Groenhof, A. R.; Ehlers, A. W.; Lammertsma, K. Validation of Exchange−Correlation Functionals for Spin States of Iron Complexes. *J. Phys. Chem. A* **2004**, *108*, 5479-5483.

(5) Harvey, J. N. On the accuracy of density functional theory in transition metal chemistry. *Annu. Rep. Prog. Chem., Sect. C: Phys. Chem* **2006**, *102*, 203-226.

(6) Ye, S.; Neese, F. Accurate Modeling of Spin-State Energetics in Spin-Crossover Systems with Modern Density Functional Theory. *Inorg. Chem.* **2010**, *49*, 772-774.

Table S1. Relative energies (in kcal·mol^{-1}) of some selected intermediates and transition states with the different levels of theory used in this contribution.

Species	B3PW91	B3PW91-D3	PBE0	PBE0-D3	M06	MP2	CCSD(T)*
1b + ethane	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS(1a-1b) + ethane	54.3	53.3	54.3	53.8	49.0	56.2	53.7
$1a^{S}$+ H2 + ethane	43.3	45.2	45.0	46.0	40.2	41.6	39.2
$1a^{T}$ + H2 + ethane	39.8	41.7	40.9	41.9	47.3	42.6	42.4
TS(1a-3a)	50.7	47.9	50.2	48.6	48.6	48.6	*n/c*
TS(1b-2)	25.2	18.9	22.4	19.0	21.6	20.7	23.6
2	10.3	3.9	7.8	4.4	4.3	3.6	*n/c*
TS(9-10)	66.2	64.3	*n/c*	*n/c*	*n/c*	60.0	62.4
TS(8-16)	48.8	37.3	*n/c*	*n/c*	*n/c*	*n/c*	42.4
TS(19-42)	79.0	71.0	*n/c*	*n/c*	*n/c*	67.3	73.3
3a	11.6	7.4	11.2	9.0	8.7	6.1	*n/c*

*Single-point energies on the B3PW91 optimized geometries

n/c: not calculated

Table S2. $(SiO)_2Ta\text{-}H_X$ main bond distances (Å) computed with the **2T** model and different levels of theory.[a] Experimental values are added for comparison.

	B3PW91	**M06**	**PBE0**	**Exp.**[2]
		1a[b]		
Ta-O	1.855	1.855	1.851	1.91
Ta-H	1.788	1.788	1.787	--
		1b		
Ta-O	1.876	1.874	1.872	1.91
Ta-H	1.748/1.750	1.751/1.754	1.746/1.748	

[a] Basis set for all calculations: LanL2TZ(*f*) for Ta and 6-311++G(*d*,*p*) for non-metal atoms

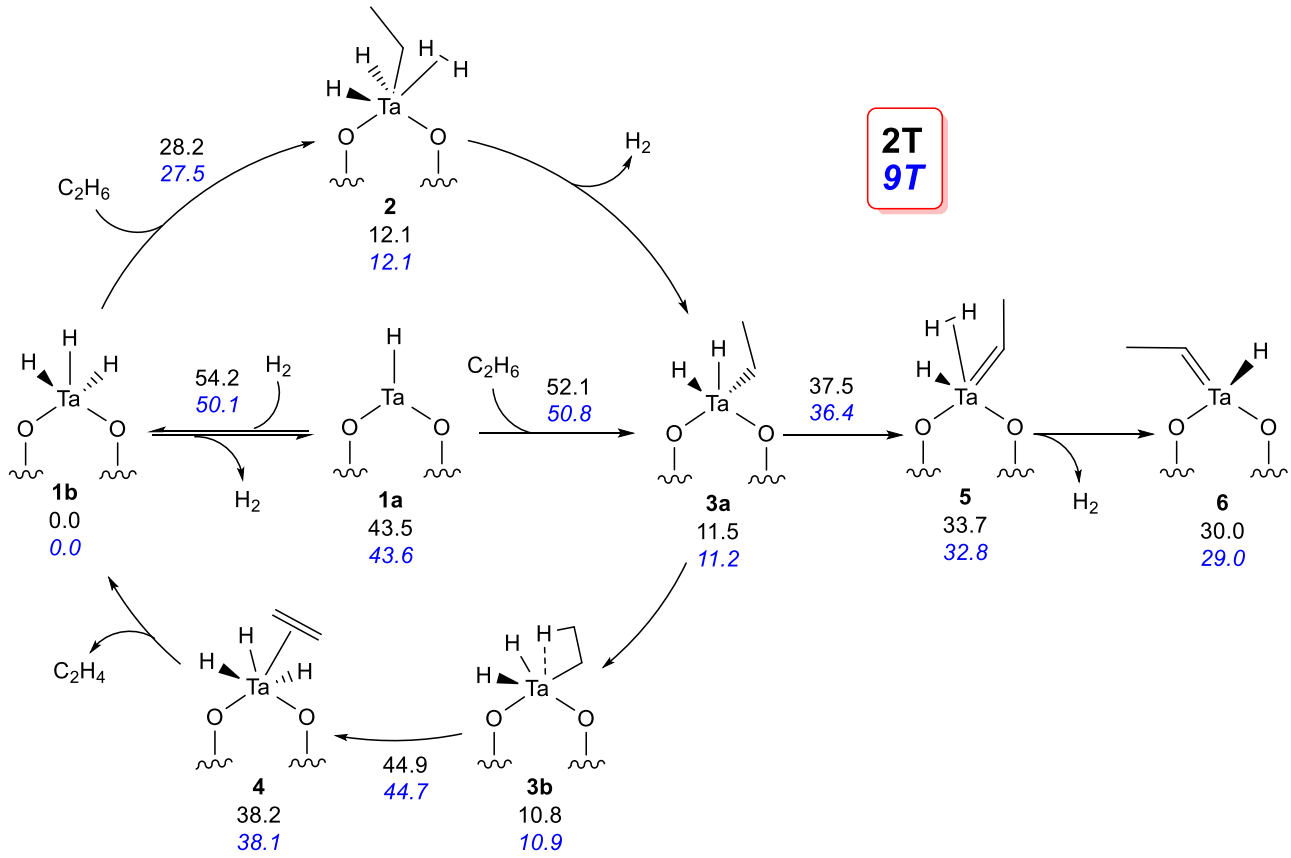
[b] Singlet state

Table S3. Ta-H stretching frequencies (cm^{-1}) of $(SiO)_2Ta\text{-}H_X$ species computed with the **2T** model and different levels of theory.[a] Experimental values are added for comparison.

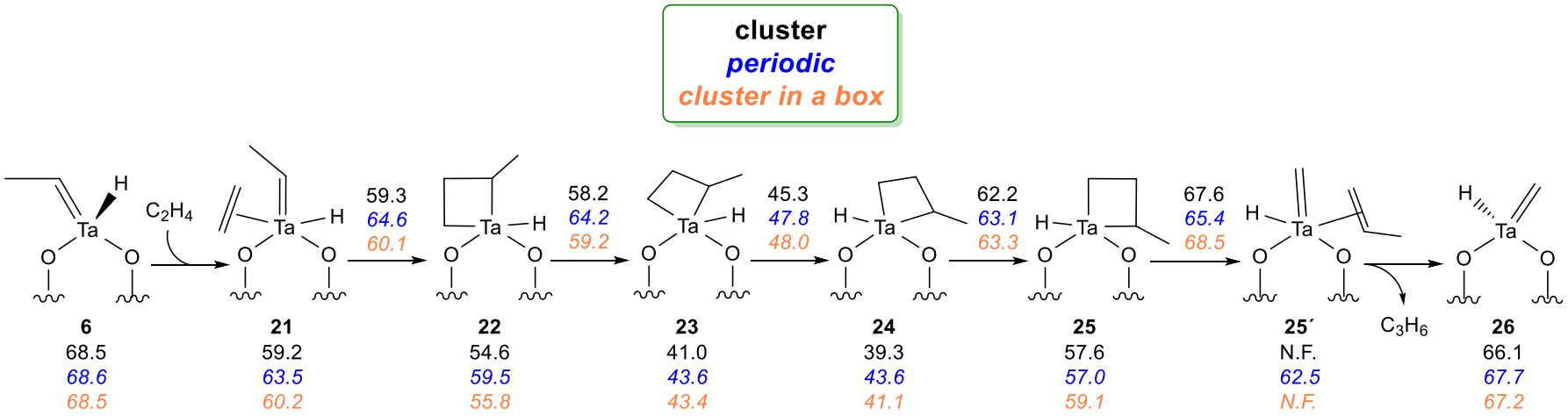
	B3PW91	**M06**	**PBE0**	**Exp.**[3]
		1a[b]		
ν (Ta-H)	1826	1774	1832	1830
		1b		
ν^{sym} (Ta-H)	1940	1894	1949	1860
ν^{asymm} (Ta-H)	1865/1896	1822/1824	1875/1906	

[a] Basis set for all calculations: LanL2TZ(*f*) for Ta and 6-311++G(*d*,*p*) for non-metal atoms

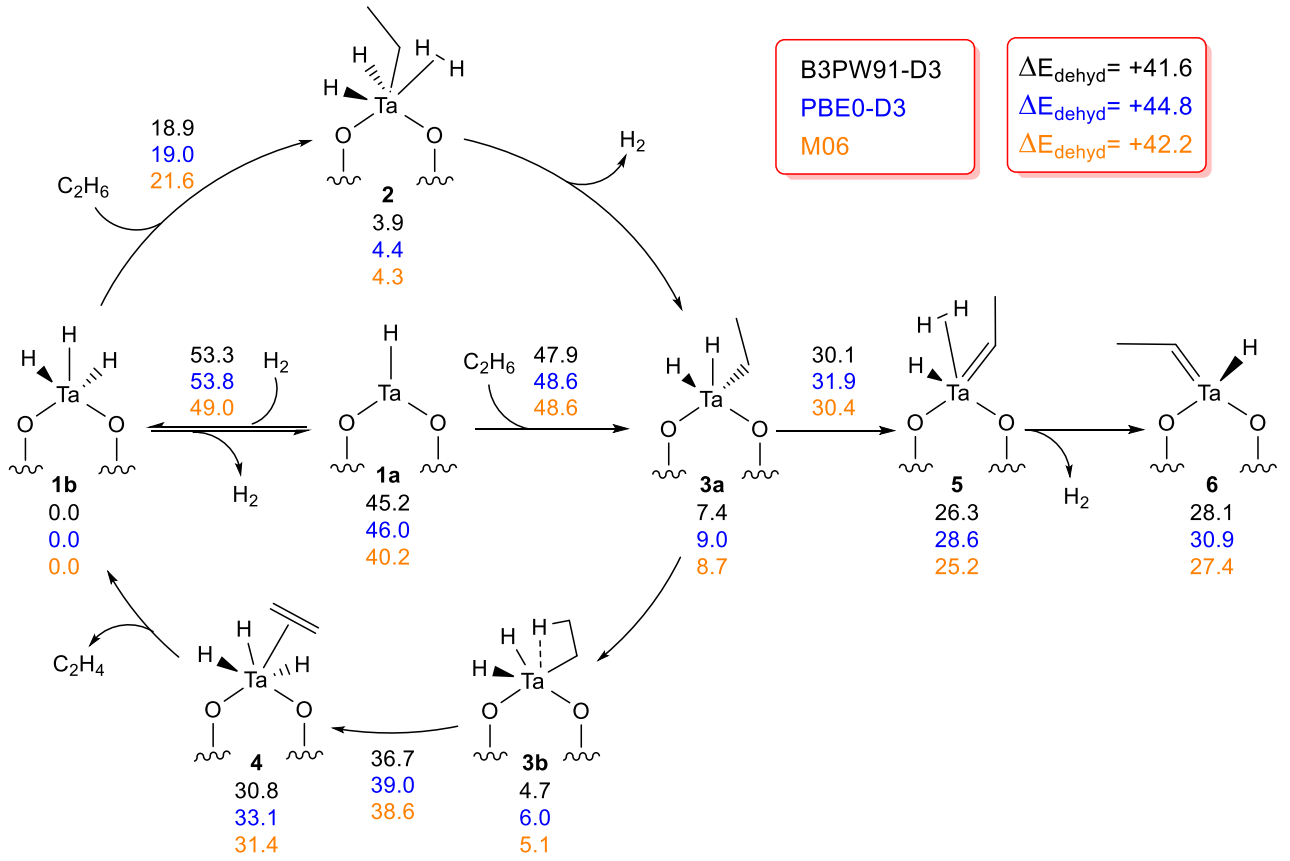
[b] Singlet state



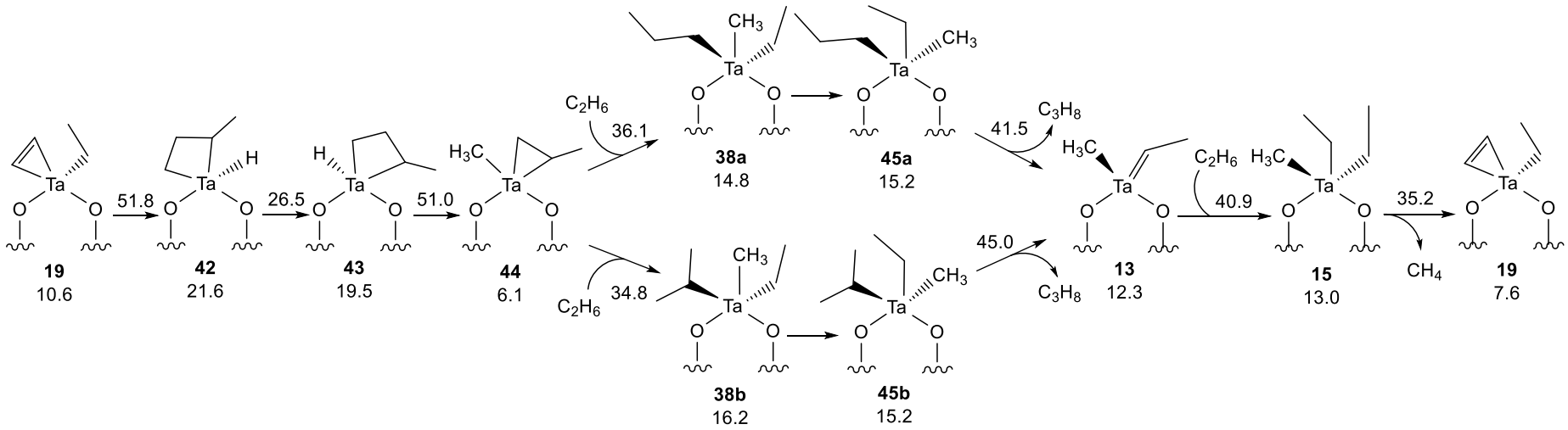
Scheme S1. Relative energies (E_{SCF}, in kcal·mol^{-1}) with respect to separated reactants of all intermediates and transition states (numbers in the arrows) involved in the C-H bond activation of ethane, ethane dehydrogenation and formation of the Ta-alkylidene-hydride **6** using **2T** (numbers in black, top) and **9T** (numbers in italic blue, bottom) cluster as silica surface models. Energies were calculated at the B3PW91 level with the LanL2TZ(*f*) RECP for Ta and the 6-31G(*d*,*p*) basis set for the rest of atoms. Optimized structures can be found in Figures S1 and S2 for **9T** and **2T**, respectively. For **1a** only the singlet state is reported.



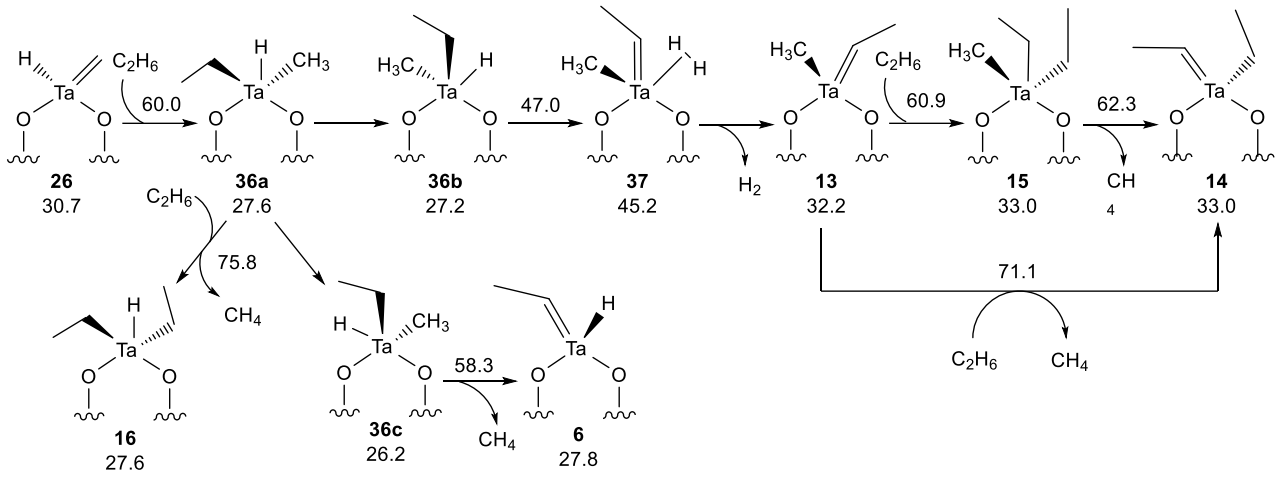
Scheme S2. Relative energies (E, in kcal·mol^{-1}) with respect to separated reactants of all intermediates and transition states (numbers in the arrows) involved in the ethene cross-metathesis using the **2T** cluster model (numbers in black, top), the periodic model (numbers in italic blue, middle) and the **2T** cluster in a 20x20x20 Å box (numbers in italic orange, bottom). Energies were calculated using the PBEPBE correlation functional for both models. The origin of the energies is the system **1b** + 2*ethane. The N.F. designation for **25´** using the cluster model indicates that this intermediate could not be found on the potential energy surface. Optimized structures can be found in Figures S3 and S4 for the cluster and periodic model, respectively.



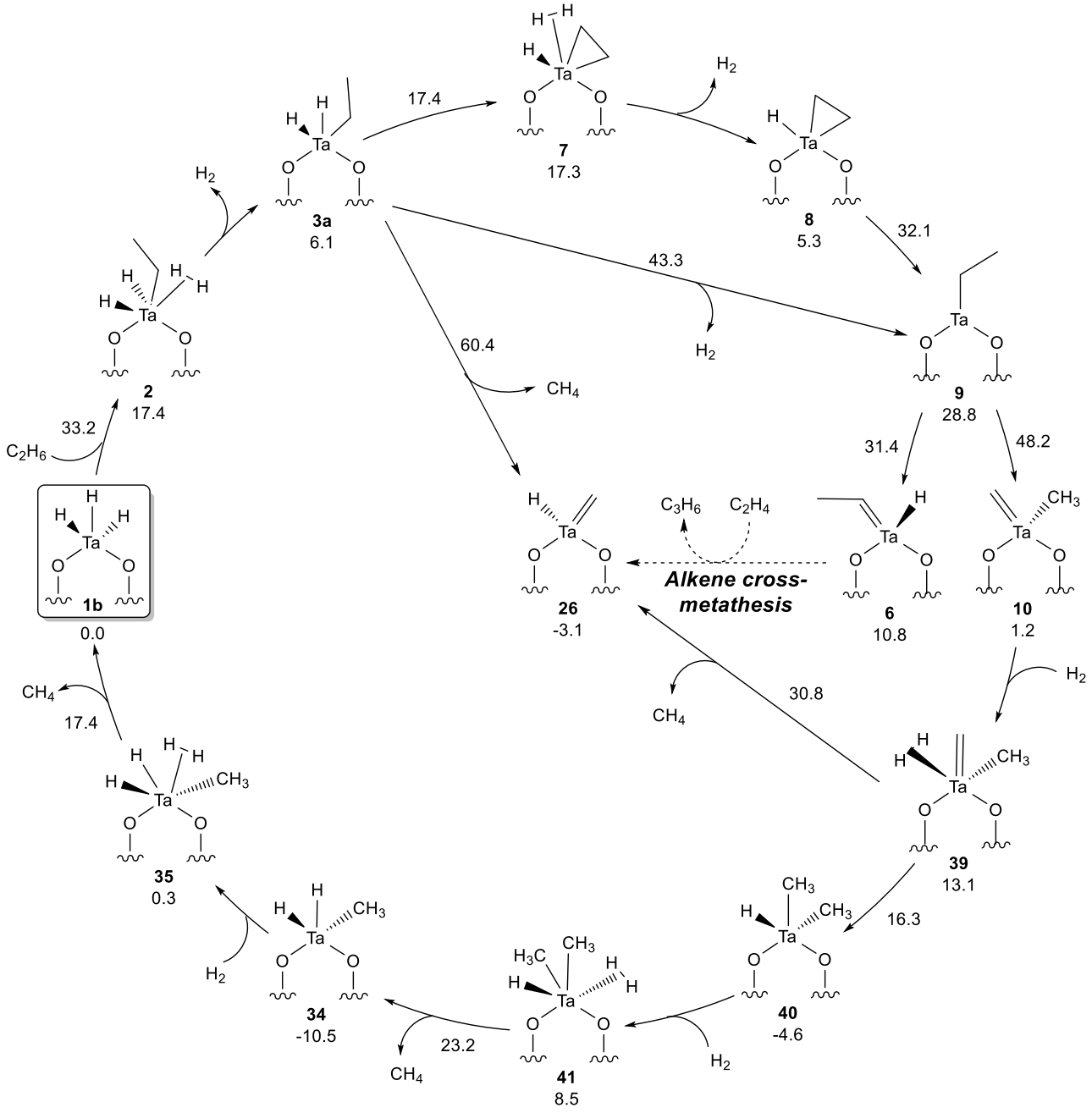
Scheme S3. Relative energies (in kcal·mol^{-1}) with respect to separated reactants of all intermediates and transition states (numbers in the arrows) involved in the activation of the C-H bond of ethane, dehydrogenation and formation of the Ta-alkylidene-hydride **6** using three different hybrid functionals: B3PW91-D3 (E+D3, in black, top), PBE0-D3 (E+D3, in blue, middle) and M06 (E, in orange, bottom). Geometries and energies were calculated using the LanL2TZ(*f*) RECP for Ta and the 6-311++G(*d*,*p*) for the rest of atoms. Optimized structures can be found in Figures S5 and S6 for PBE0 and M06, respectively. Optimized structures for the B3PW91 are found in the main manuscript. For **1a** only the singlet state is reported.



Scheme S4. Relative Gibbs energies ($\Delta G_{423,}$ in kcal·mol^{-1}) with respect to separated reactants of the intermediates and transition states (numbers in the arrows) associated with the ethane metathesis reaction involving **19** as catalyst. Optimized structures can be found in Figures S12. Though most of the steps shows similar barriers to those reported in the manuscript, the conversion from **19** to **42** and from **43** to **44** are energetically demanding. These high energy barriers indicate that these processes do not take place during formation of methane and propane as main products of metathesis of ethane.



Scheme S5. Relative Gibbs energies (ΔG_{423}, in kcal·mol^{-1}) with respect to separated reactants of all intermediates and transition states (numbers in the arrows) involved in the formation of methane from **26** by reaction with ethane. Optimized structures can be found in Figures S15.



Scheme S6. Full catalytic cycle for hydrogenolysis of ethane by **1b**. Relative Gibbs energies (ΔG_{423}) with respect to separated reactants are given in kcal·mol^{-1}. Optimized structures of most intermediates and transitions states are already presented in the main manuscript. Other structures are shown in Figure S17.

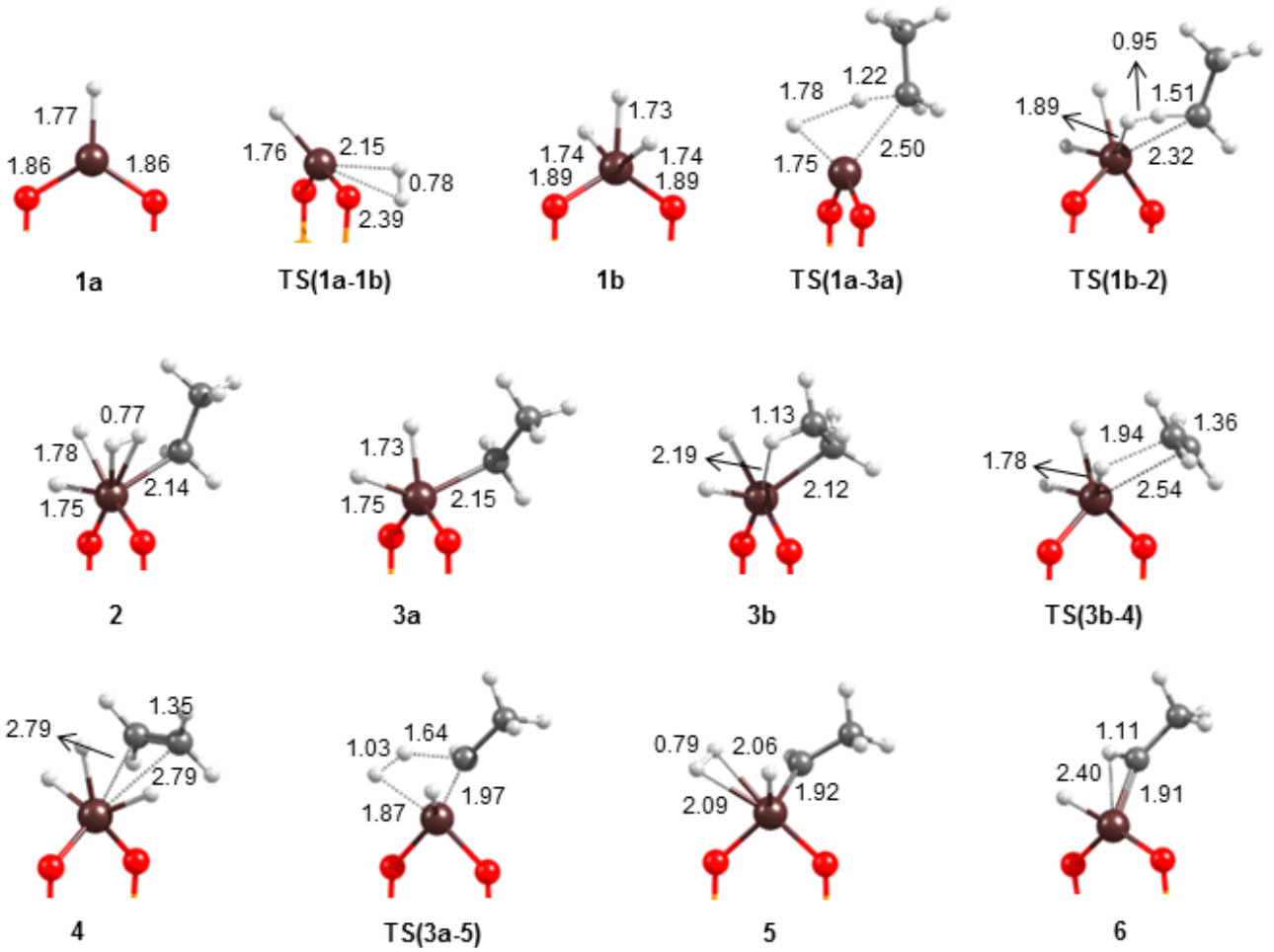


Figure S1. B3PW91 optimized geometries of all minima and transition states involved in the C-H bond activation of ethane, ethane dehydrogenation and formation of the Ta-alkylidene-hydride **6** with the **9T** cluster models. Geometries were obtained with the LanL2TZ(*f*) RECP for Ta and the 6-31G(*d*,*p*) basis set for the rest of atoms. For **1a** only the singlet state is reported. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

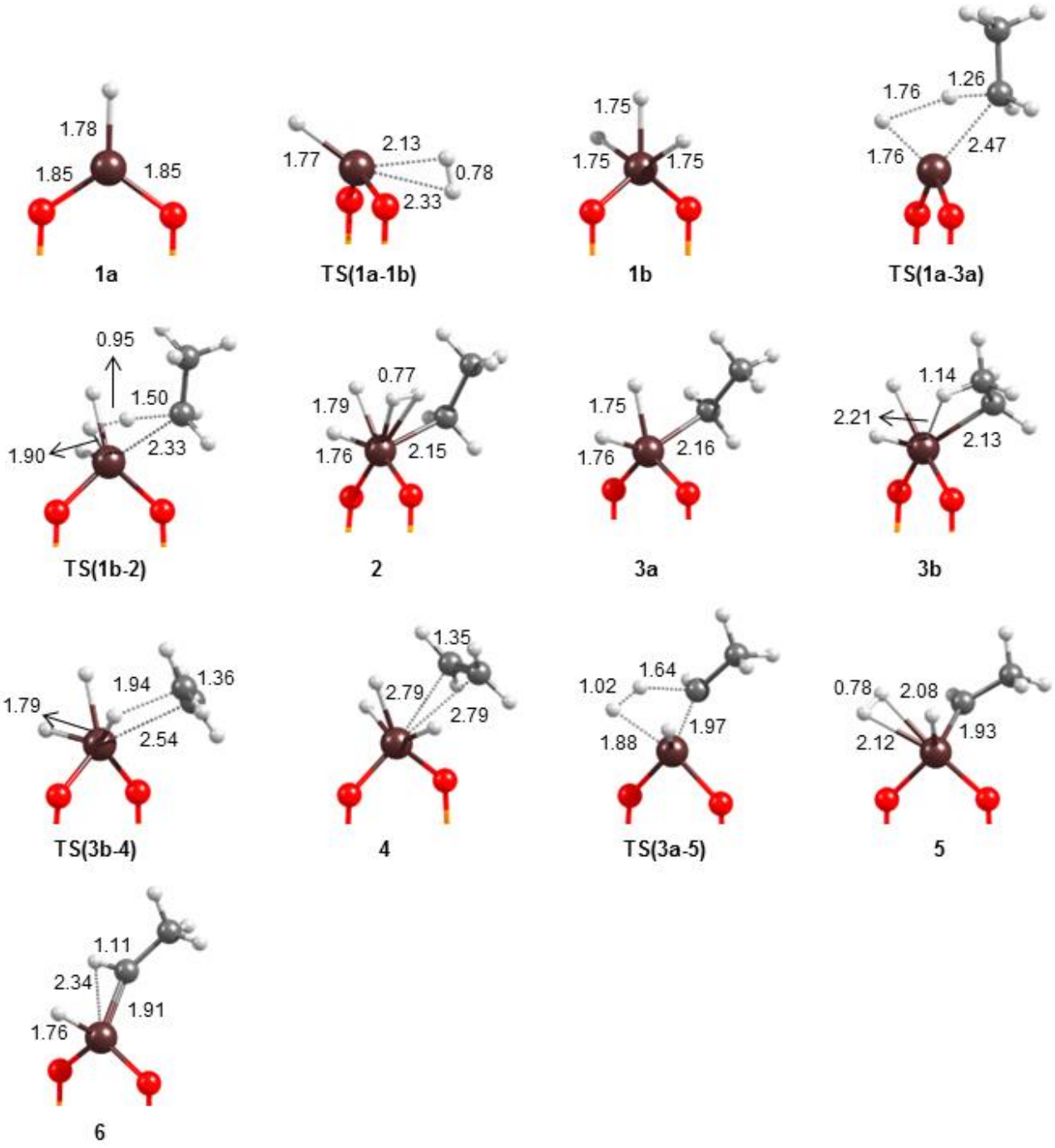


Figure S2. B3PW91 optimized geometries of all minima and transition states involved in the C-H bond activation of ethane, ethane dehydrogenation and formation of the Ta-alkylidene-hydride **6** with the **2T** cluster models (to allow comparison with the **9T** models). Geometries were obtained with the LanL2TZ(*f*) RECP for Ta and the 6-31G(*d,p*) basis set for the rest of atoms. For **1a** only the singlet state is reported. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

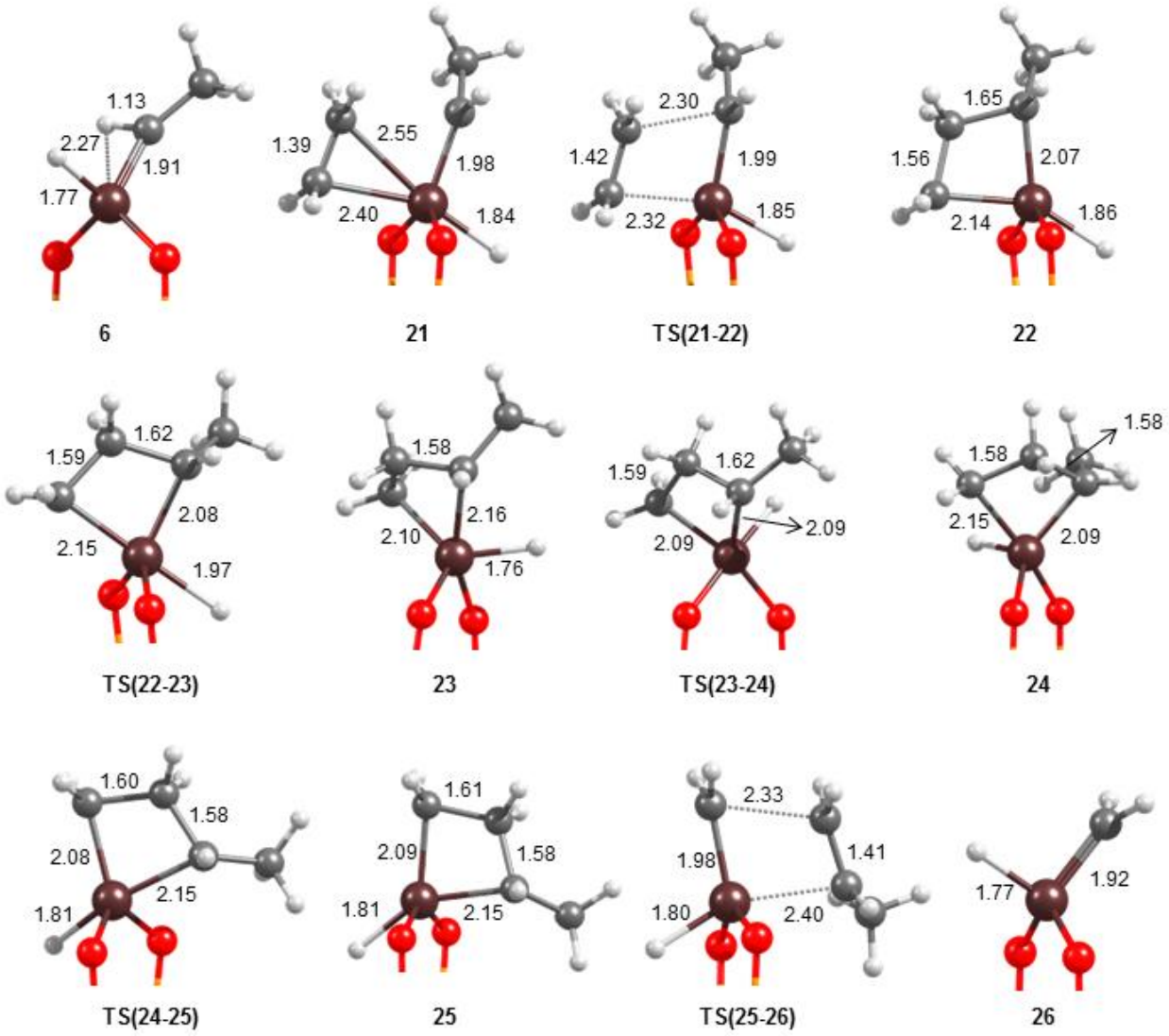


Figure S3. PBE optimized geometries of all minima and transition states involved in the ethene cross-metathesis using the **2T** cluster. Geometries were obtained with the LanL2TZ(*f*) RECP for Ta and the 6-311++G(*d*,*p*) basis set for the rest of atoms. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

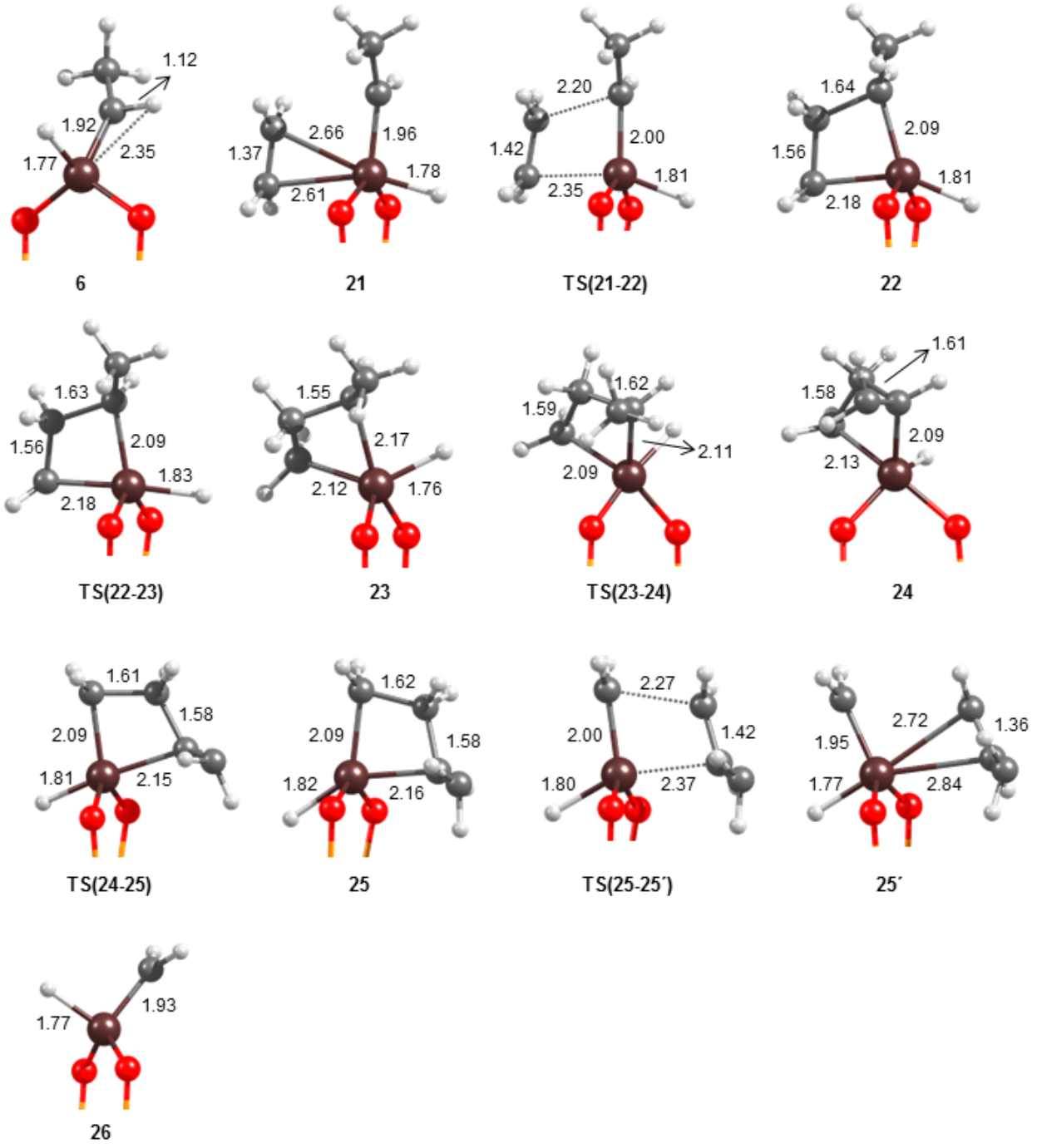


Figure S4. PBE optimized geometries of all minima and transition states involved in the ethene cross-metathesis using the model based on periodic boundary conditions (PBC) and the PAW formalism. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

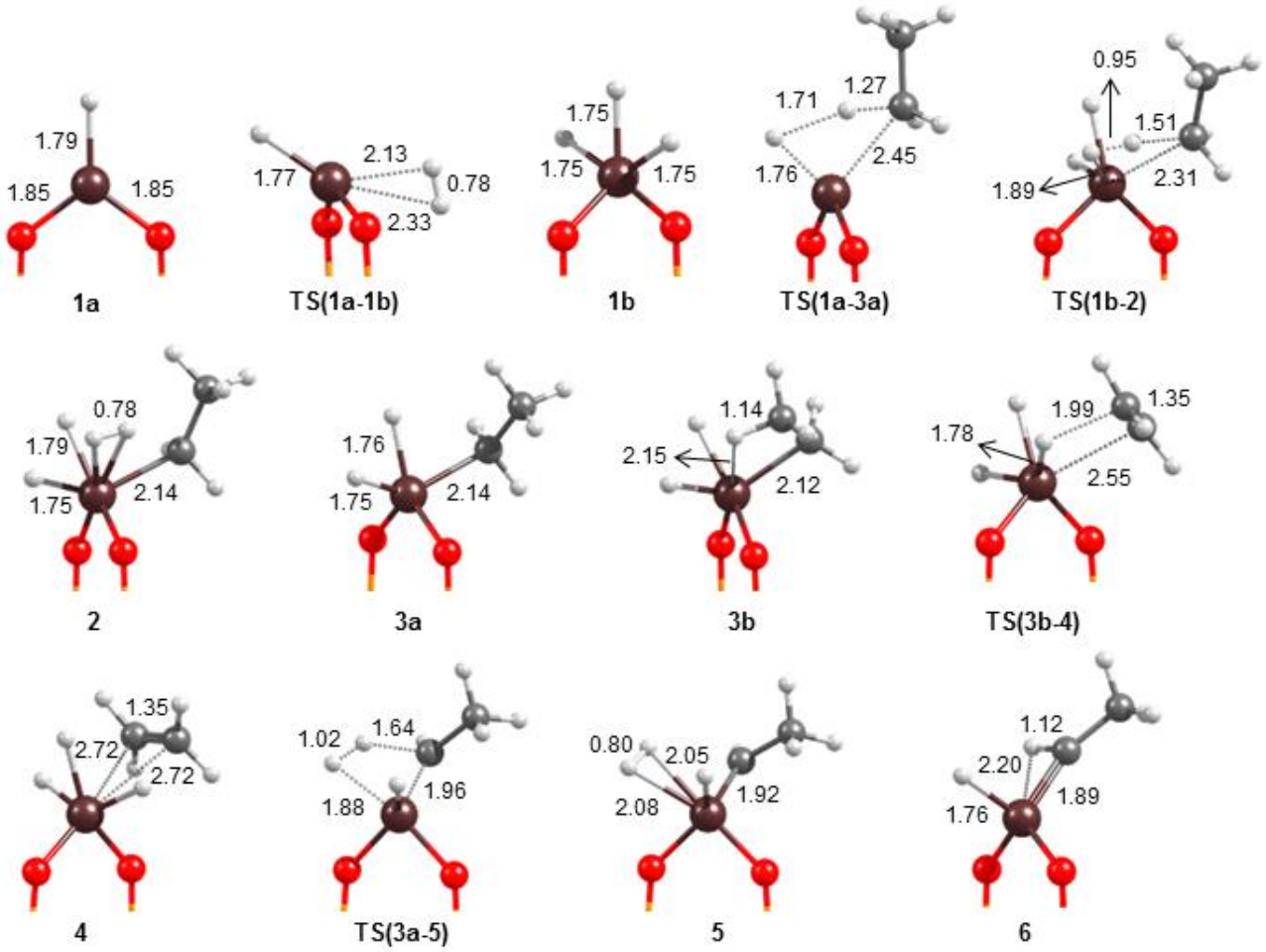


Figure S5. PBE0 optimized geometries of all minima and transition states involved in the C-H bond activation of ethane, ethane dehydrogenation and formation of Ta-alkylidene-hydride **6** using the **2T** cluster model. Geometries were obtained using the LanL2TZ(*f*) RECP for Ta and the 6-311++G(*d*,*p*) for the rest of atoms. For **1a** only the singlet state is reported. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

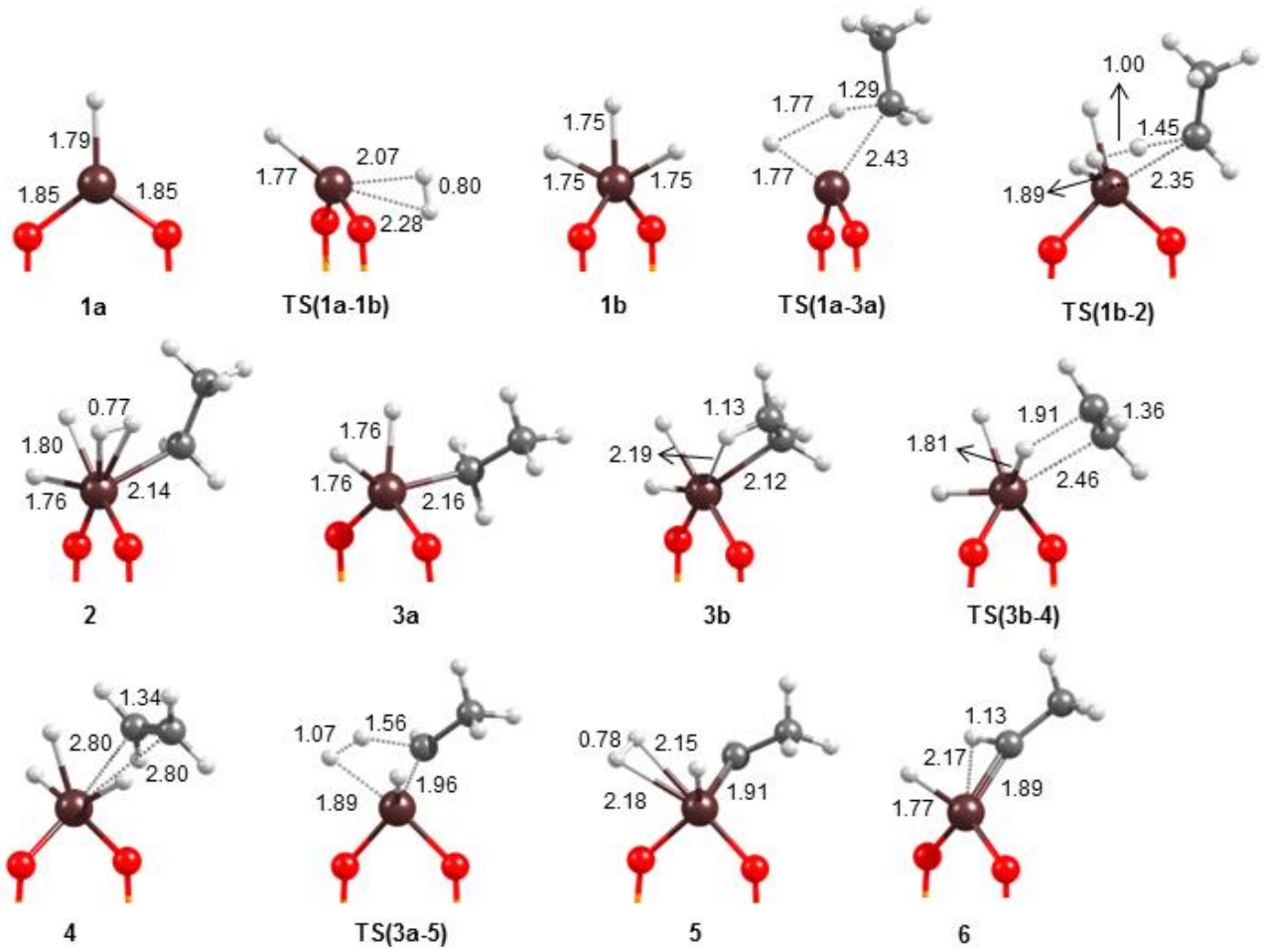


Figure S6. M06 optimized geometries of all minima and transition states involved in the C-H bond activation of ethane, ethane dehydrogenation and formation of Ta-alkylidene-hydride **6** using the **2T** cluster model. Geometries were calculated using the LanL2TZ(*f*) RECP for Ta and the 6-311++G(*d*,*p*) for the rest of atoms. For **1a** only the singlet state is reported. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

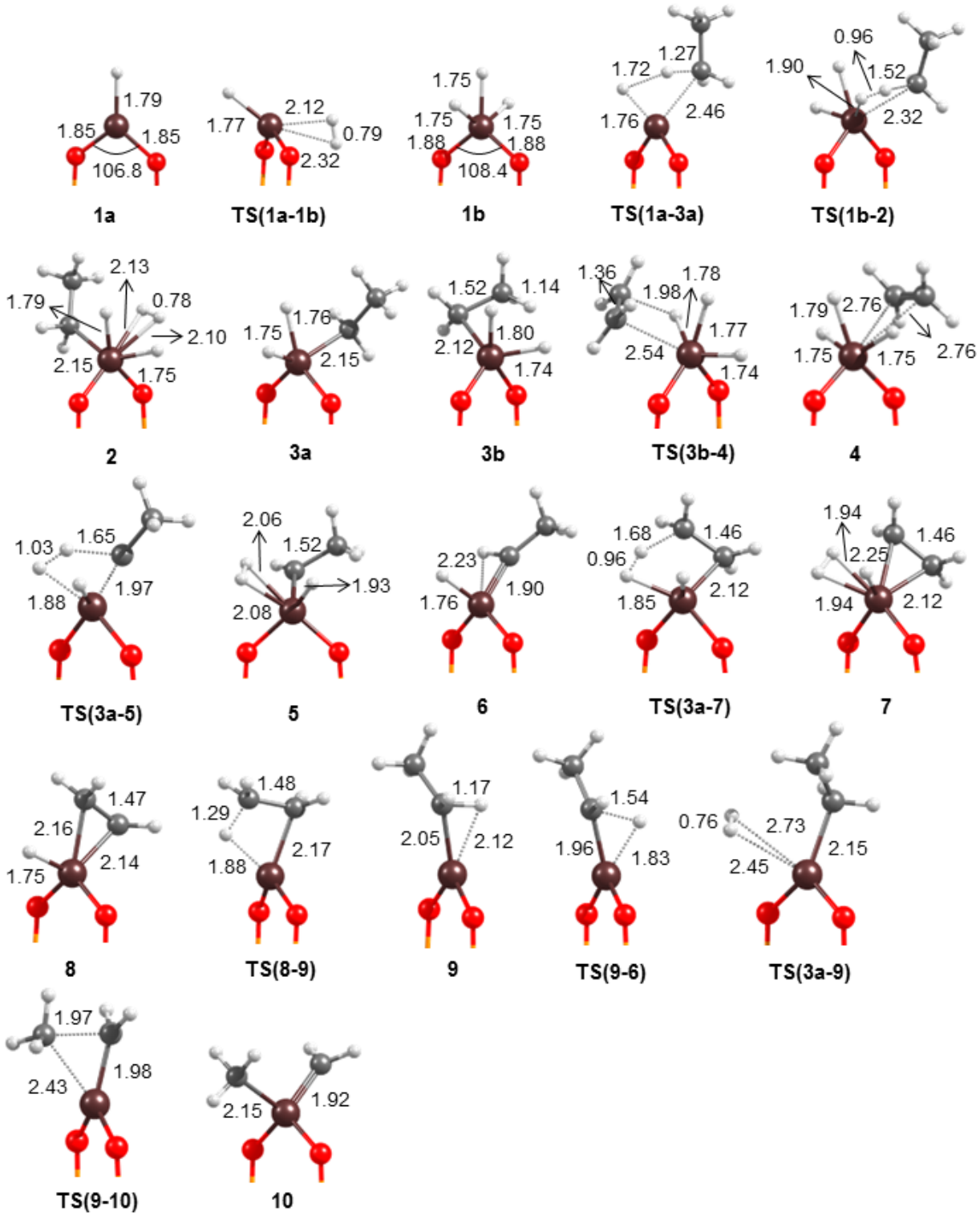


Figure S7. B3PW91 optimized geometries of all minima and transition states involved in the C-H bond activation of ethane, ethane dehydrogenation and formation of Ta-alkylidene-hydrides **6** and **10**. For **1a** and **9** only the singlet state is reported. Distances are given in Å and angles in degrees. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

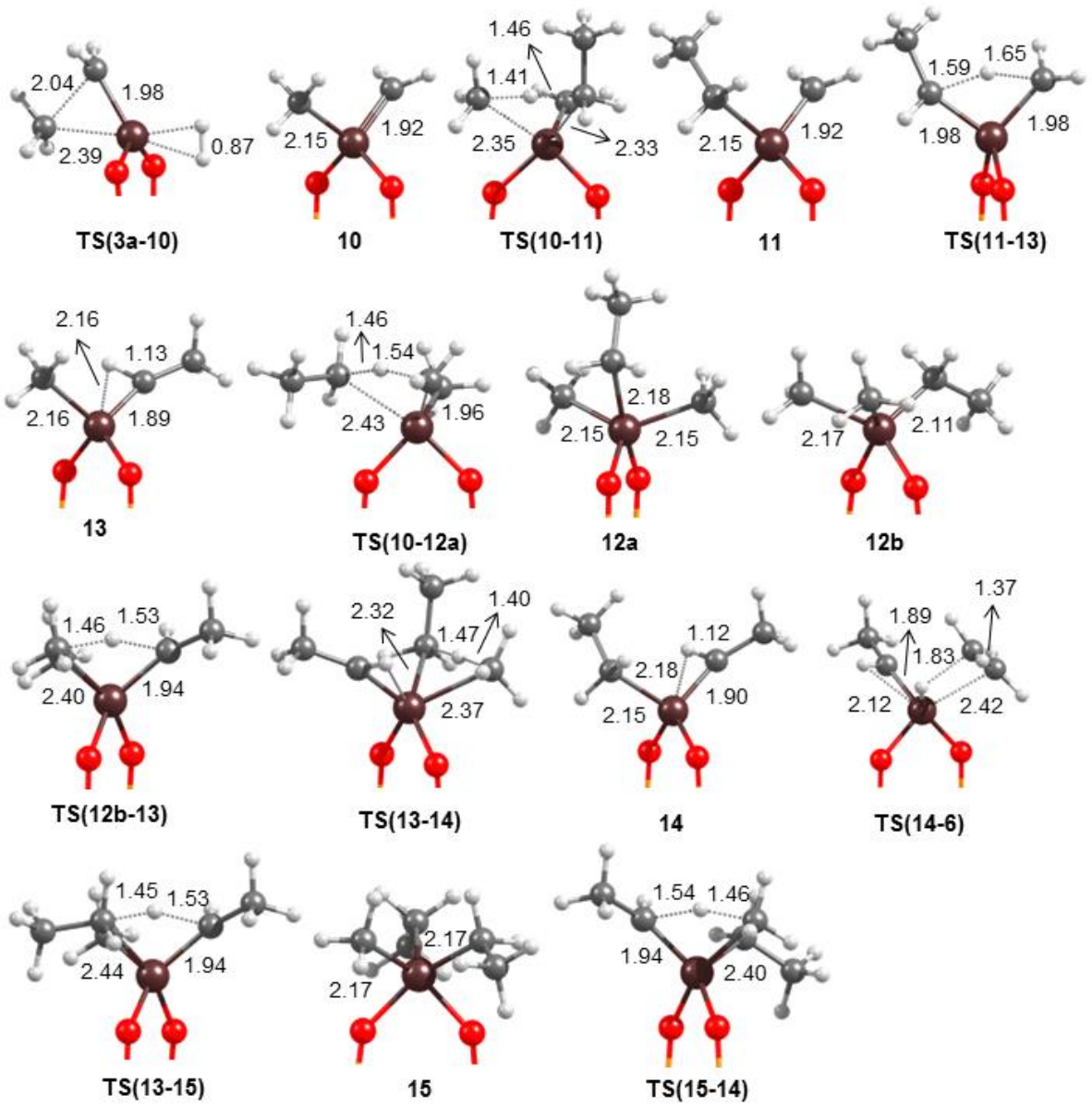


Figure S8. B3PW91 optimized geometries of all minima and transition states involved in the reaction of Ta-alkylidene **10** with ethane. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

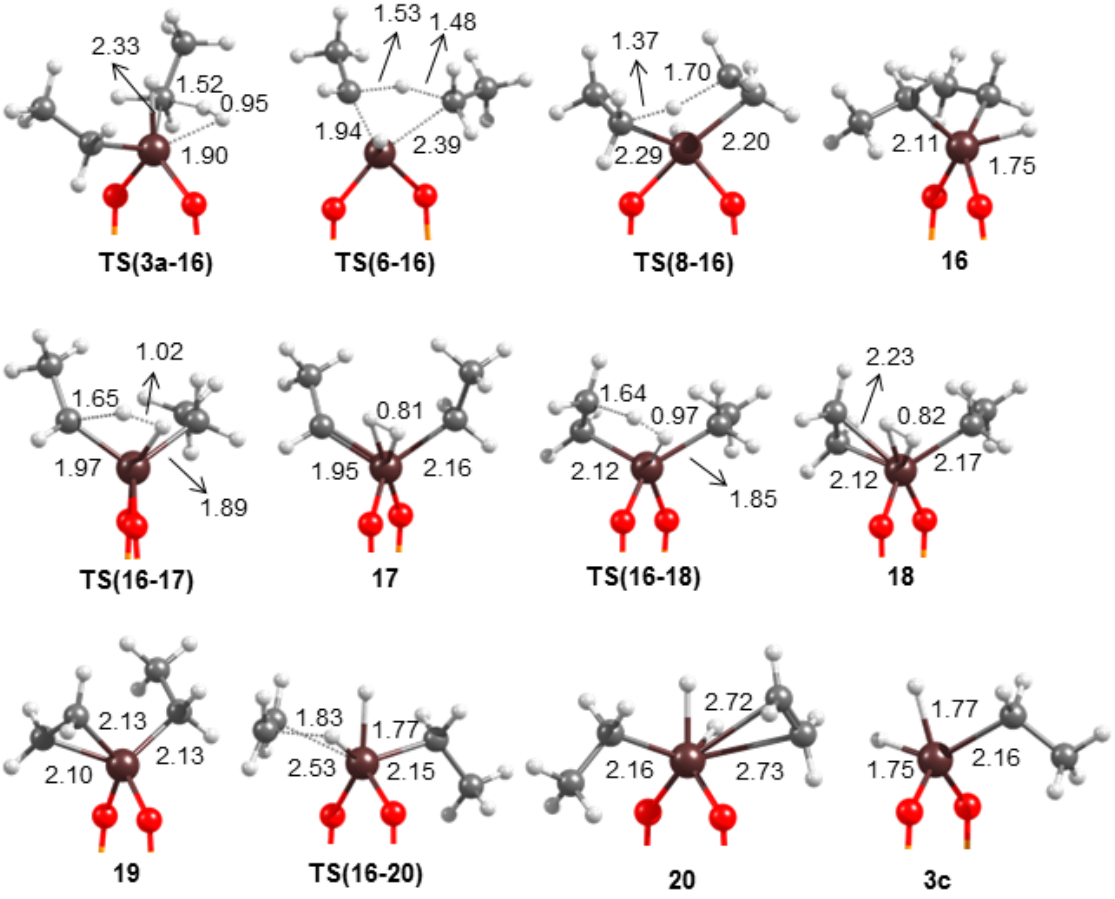


Figure S9. B3PW91 optimized geometries of all minima and transition states involved in the reaction of Ta-alkyl **3a** with ethane. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

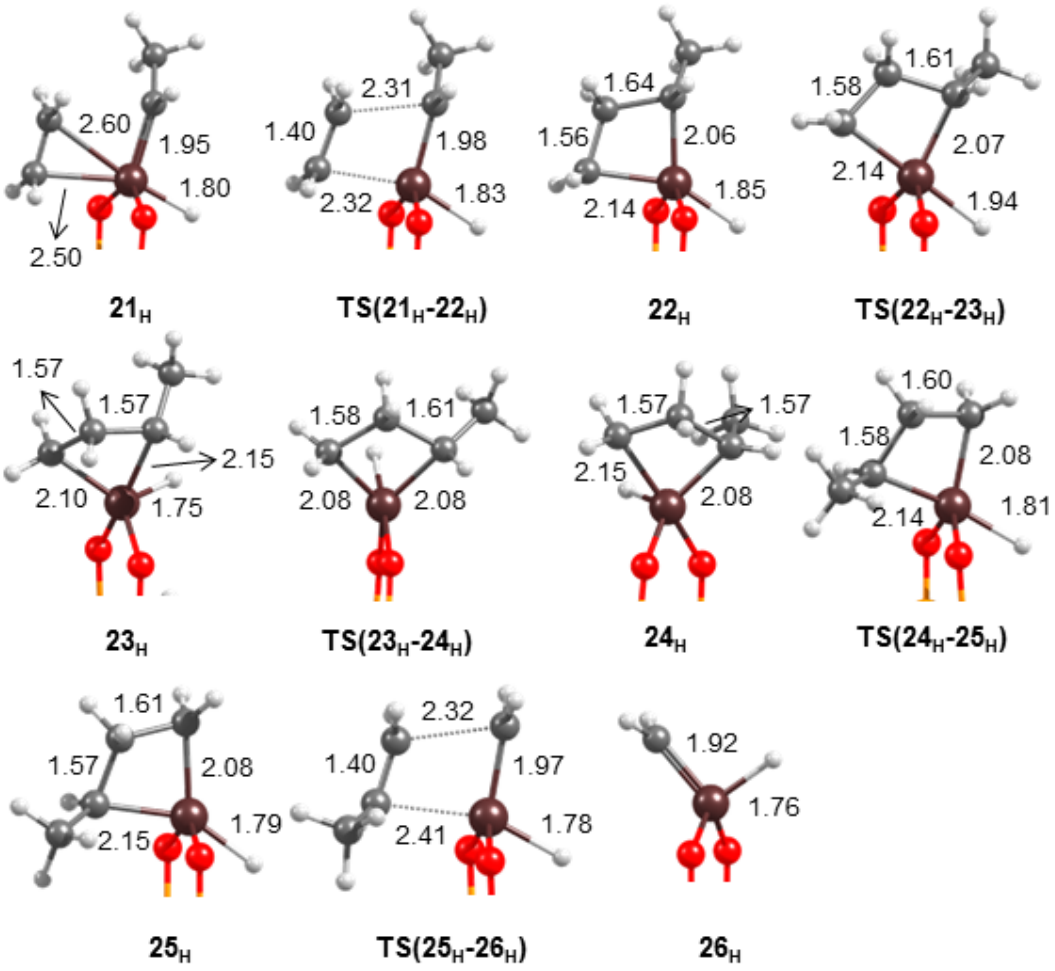


Figure S10. B3PW91 optimized geometries of all minima and transition states involved in the reactivity of Ta-alkylidene-hydride **6** with ethene. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

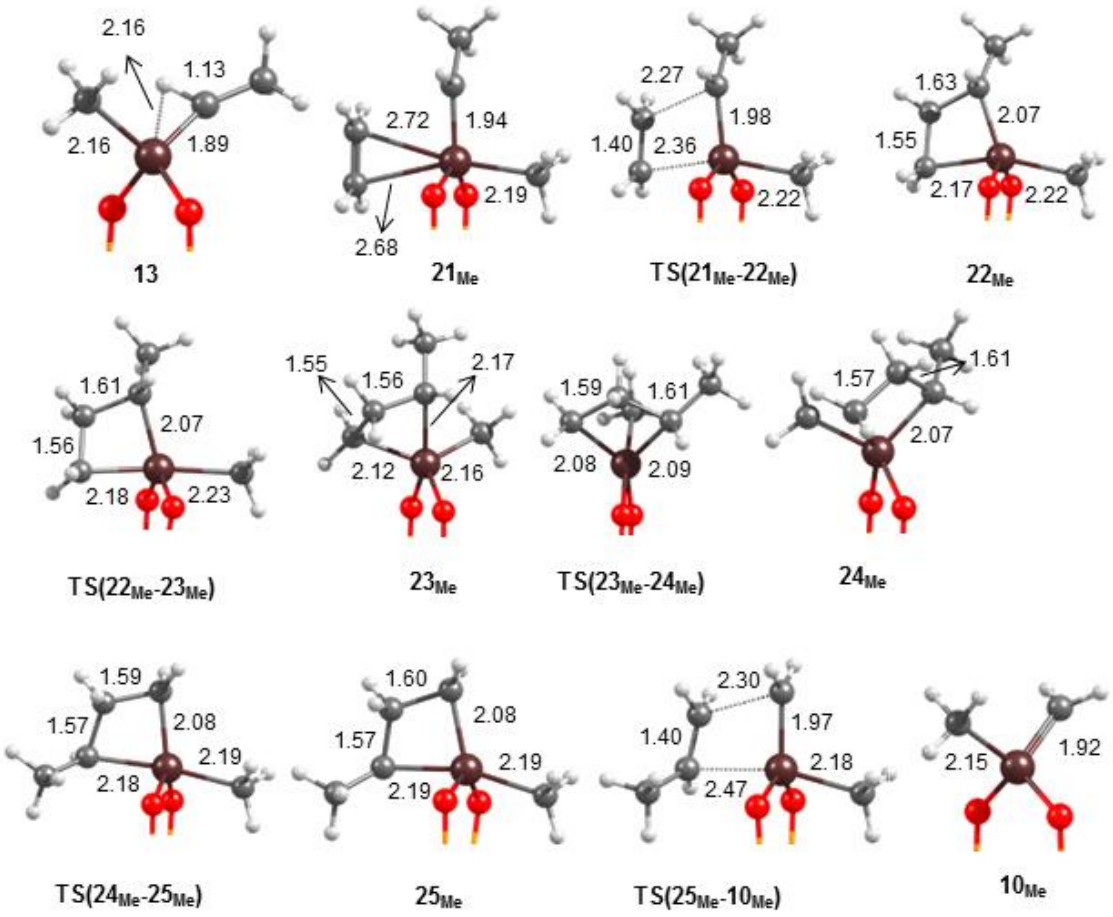


Figure S11. B3PW91 optimized geometries of all minima and transition states involved in the reactivity of Ta-methyl-alkylidene **13** with ethene. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

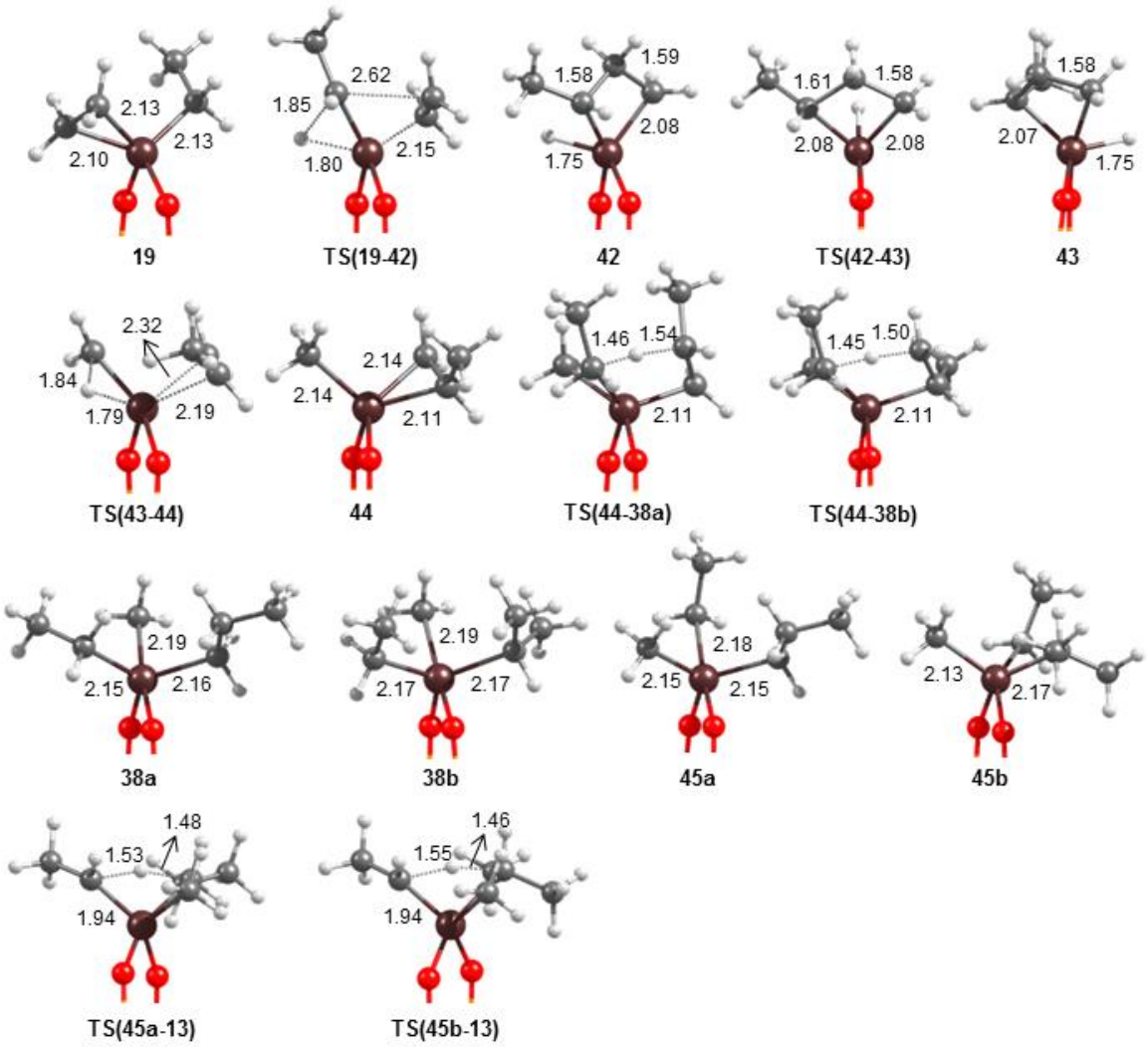


Figure S12. B3PW91 optimized geometries of the minima and transition states involved in the reactivity of **19** with ethane to form methane and propane. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

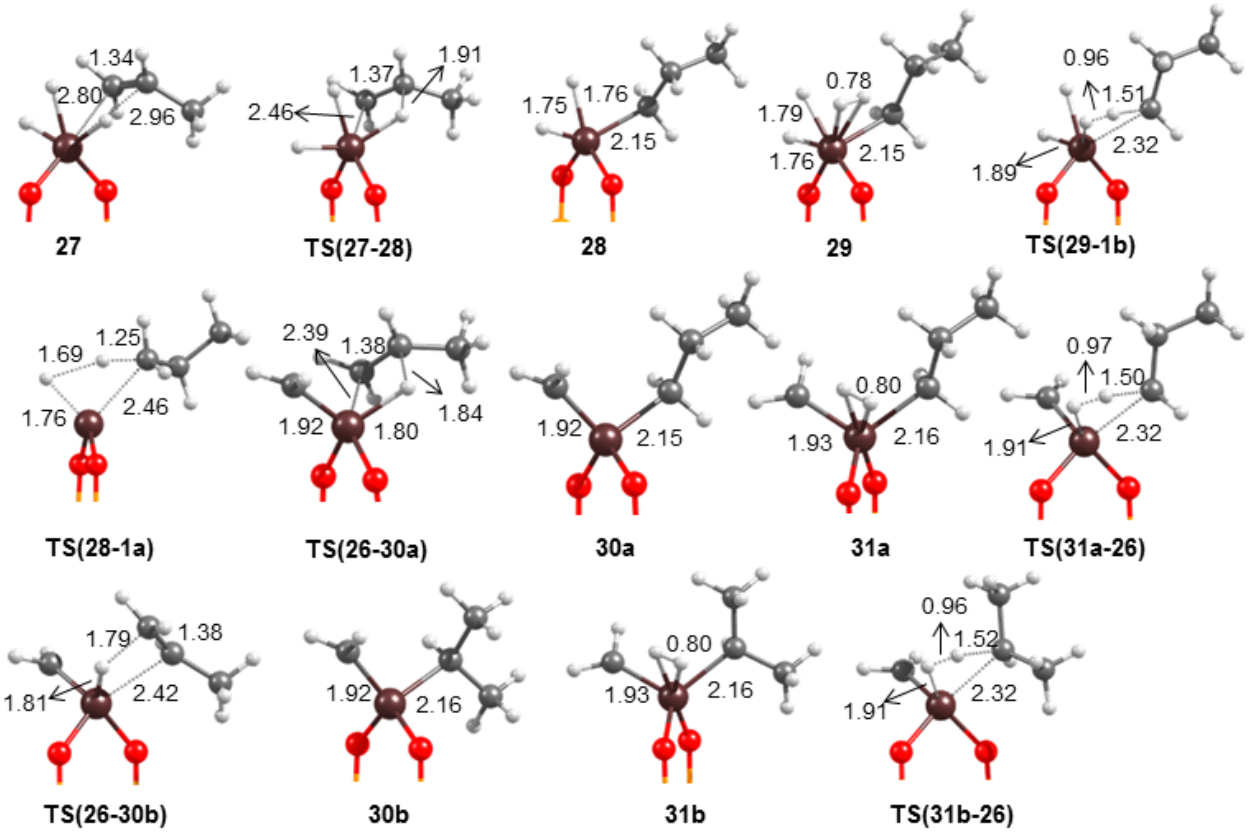


Figure S13. B3PW91 optimized geometries of all minima and transition states involved in the hydrogenation of propene by **1b** and **26** and H_2. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

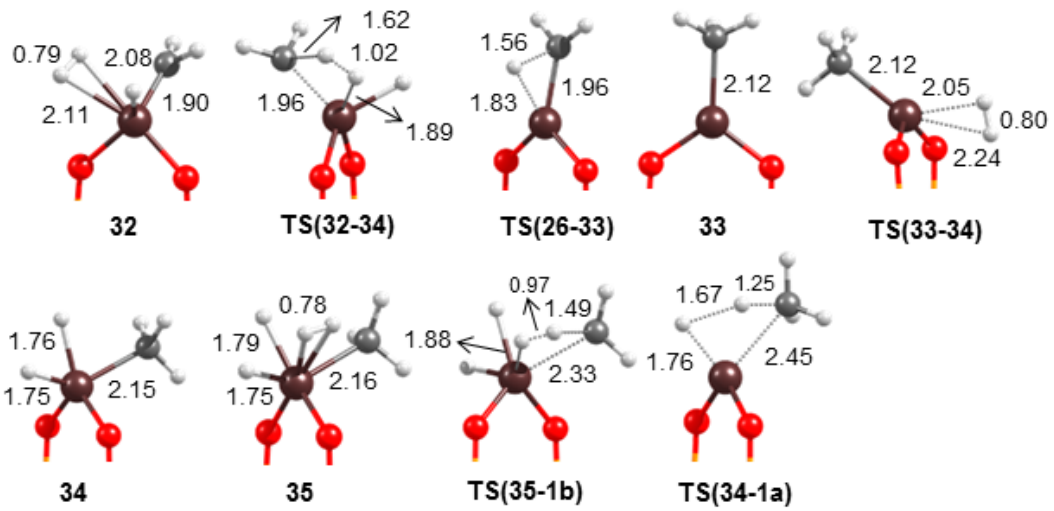


Figure S14. B3PW91 optimized geometries of all minima and transition states involved in the hydrogenation of **26** to obtain methane. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

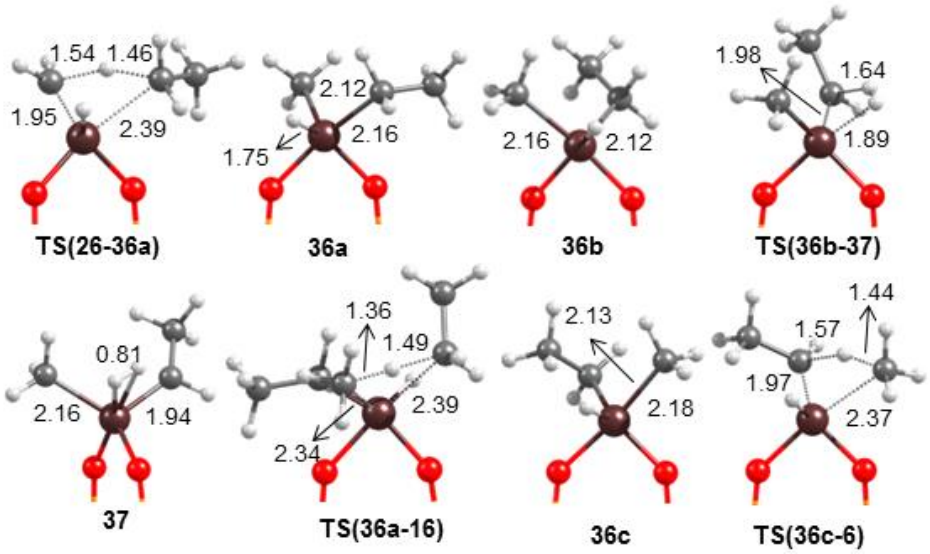


Figure S15. B3PW91 optimized geometries of all minima and transition states involved in the reaction of **26** with ethane to obtain methane. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

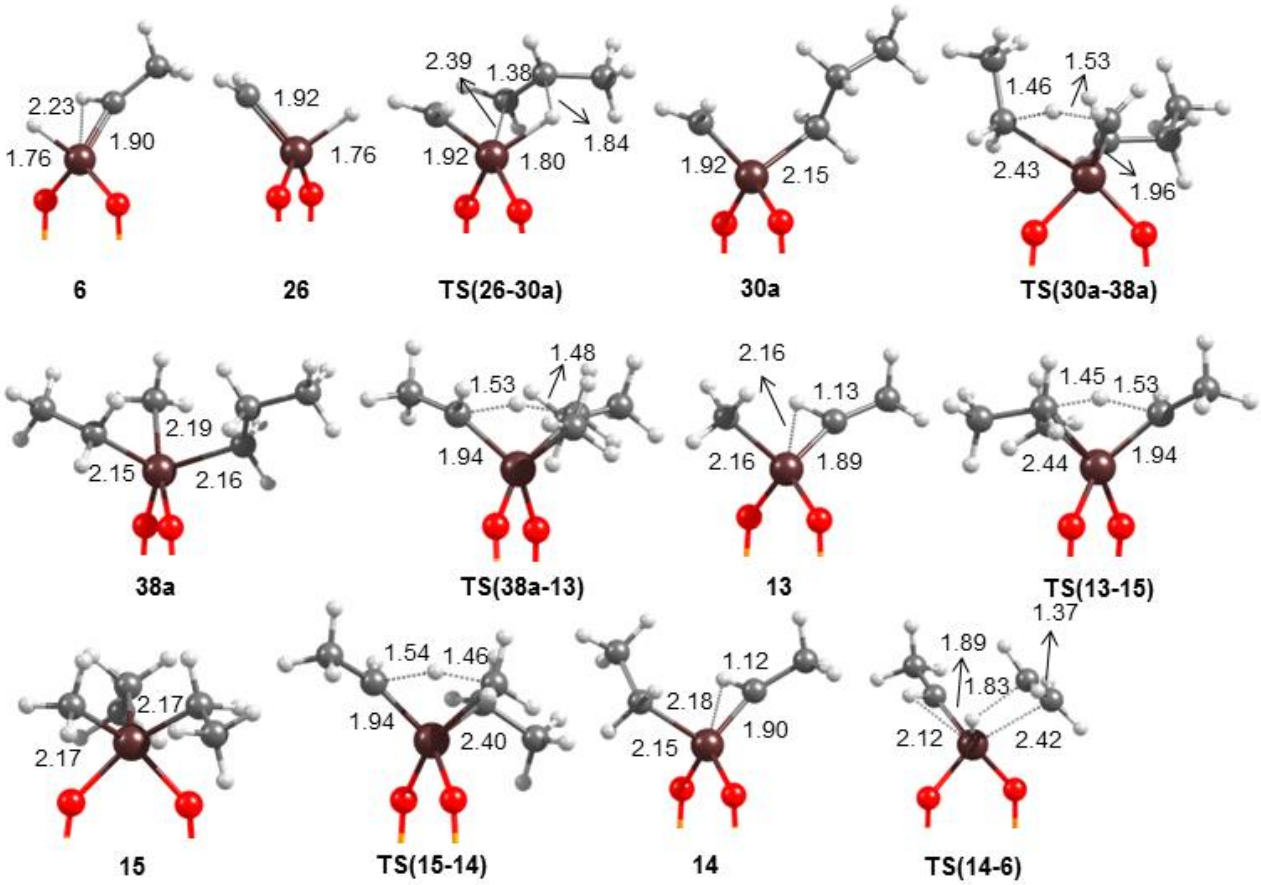


Figure S16. B3PW91 optimized geometries of most important minima and transition states involved in ethane metathesis involving **14** as catalyst. Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

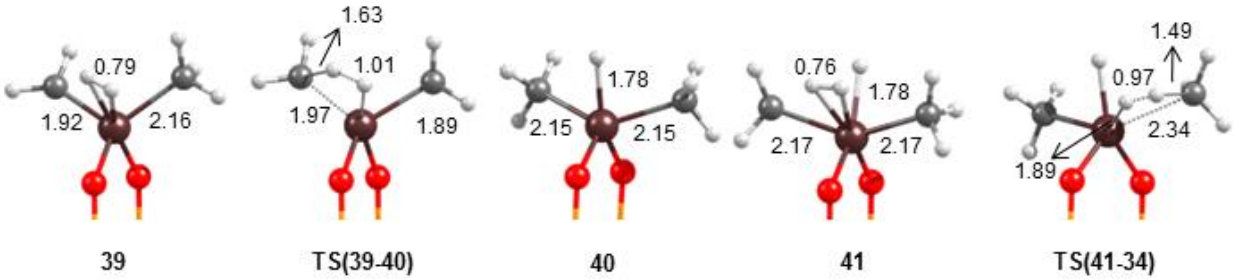


Figure S17. B3PW91 optimized geometries of the minima and transition states involved in the hydrogenolysis of ethane by TaH_x/SiO_2 (x=1, 3). Distances are given in Å. Color code of the elements is as follows: Ta: brown, O: red, C: gray, H: white.

Cartesian coordinates and absolute energies of all stationary points reported in the manuscript and ESI

I. Reactants, products and by-products

Ethane

C	0.000000	0.000000	0.762261
H	-0.508935	0.882220	1.161755
H	1.018493	-0.000359	1.161755
H	-0.509558	-0.881861	1.161755
C	0.000000	0.000000	-0.762261
H	0.509558	-0.881861	-1.161755
H	-1.018493	-0.000360	-1.161755
H	0.508935	0.882221	-1.161755

E_{SCF}= -79,825419 au
G_{423}= -79,783711 au
E_{disp}= -3,3570 kcal·mol^{-1}

Methane

C	0.000000	0.000000	0.000000
H	0.629915	0.629915	0.629915
H	-0.629915	-0.629915	0.629915
H	-0.629915	0.629915	-0.629915
H	0.629915	-0.629915	-0.629915

E_{SCF}= -40,517381 au
G_{423}= -40,499263 au
E_{disp}= -1,1731 kcal·mol^{-1}

Propane

C	1.271952	-0.258874	0.000004
H	2.169632	0.366425	-0.000068
H	1.317312	-0.905385	-0.882811
H	1.317365	-0.905259	0.882909
C	0.000000	0.583861	-0.000023
H	0.000003	1.244095	0.875463
H	-0.000003	1.244043	-0.875551
C	-1.271952	-0.258874	0.000012
H	-1.317336	-0.905292	0.882895
H	-2.169632	0.366425	-0.000006
H	-1.317340	-0.905351	-0.882826

E_{SCF}= -119,135375 au
G_{423}= -119,071742 au
E_{disp}= -6,2086 kcal·mol^{-1}

Hydrogen molecule

H	0.000000	0.000000	0.372686
H	0.000000	0.000000	-0.372686

E_{SCF}= -1,178577 au
G_{423}= -1,186474 au
E_{disp}= -0,0860 kcal·mol^{-1}

Ethene

C	-0.663809	0.000000	0.000004
C	0.663809	0.000000	-0.000003
H	-1.234747	-0.923720	-0.000010
H	-1.234747	0.923720	0.000023
H	1.234747	0.923720	0.000011
H	1.234747	-0.923720	-0.000023

E_{SCF}= -78,580470 au
G_{423}= -78,563192 au
E_{disp}= -2,4368 kcal·mol^{-1}

Propene

C	-0.131271	0.452738	0.000030
C	-1.278986	-0.220102	-0.000026
H	-0.164070	1.542023	0.000063
H	-1.301063	-1.306956	-0.000079
H	-2.236836	0.289664	-0.000031
C	1.230784	-0.163730	0.000071
H	1.178115	-1.255327	-0.000160
H	1.805058	0.152025	-0.878385
H	1.804791	0.151634	0.878850

E_{SCF}= -117,896331 au
G_{423}= -117,855181 au
E_{disp}= -5,0271 kcal·mol^{-1}

II. Activation of C-H bond of ethane, dehydrogenation and formation of Ta-alkylidene-hydrides 6 and 10

1a (singlet)

Ta	1.478635	0.000082	0.000843
O	0.372832	-1.489093	0.009584
O	0.372767	1.489212	-0.007970
Si	-1.291540	-1.542988	-0.010111
Si	-1.291613	1.542994	0.011352
O	-1.850788	-0.000014	0.001107
O	-1.883827	-2.244991	1.342490
H	-1.665463	-3.162545	1.514663
O	-1.688433	-2.343120	-1.378635
H	-2.601675	-2.339008	-1.669904
O	-1.883614	2.244070	-1.341861
H	-1.664862	3.161373	-1.514870
O	-1.688908	2.343957	1.379262

H	-2.602162	2.339674	1.670489
H	3.266658	0.000113	0.000706

E_{SCF}= -1166,752675 au
G_{423}= -1166,743600 au
E_{disp}= -19,7681 kcal·mol^{-1}

TS(1a-1b)

Ta	1.371621	-0.121658	0.060752
O	0.614009	1.587761	-0.190377
O	0.311266	-1.674752	-0.106760
Si	-1.040315	1.666880	-0.014024
Si	-1.334402	-1.454353	-0.004477
O	-1.659928	0.149723	-0.205042
O	-1.717557	2.541107	-1.220523
H	-1.482161	3.467587	-1.294164
O	-1.321462	2.290085	1.472196
H	-2.198463	2.208928	1.850708
O	-1.939501	-1.856888	1.463624
H	-1.798675	-2.746994	1.791060
O	-1.970642	-2.333258	-1.228294
H	-2.913603	-2.276689	-1.391728
H	0.657871	-0.116274	-2.151022
H	1.435605	-0.184564	-2.053183
H	2.513029	-0.199924	1.415478

E_{SCF}= -1167,913751 au
G_{423}= -1167,890051 au
E_{disp}= -22,7585 kcal·mol^{-1}

1b

Ta	1.444693	-0.000045	0.000113
O	0.348588	-1.521933	0.020262
O	0.348711	1.521930	-0.020060
Si	-1.314745	-1.556597	-0.003389
Si	-1.314621	1.556724	0.003550
O	-1.839123	0.000085	0.000045
O	-1.924193	-2.235660	1.352478
H	-1.711720	-3.150899	1.544038
O	-1.719257	-2.345228	-1.375071
H	-2.639215	-2.378624	-1.642530
O	-1.923975	2.235888	-1.352307
H	-1.711467	3.151134	-1.543796
O	-1.719105	2.345338	1.375252
H	-2.639050	2.378680	1.642761
H	3.194891	-0.000110	0.000140
H	2.184305	0.012930	1.583878
H	2.184354	-0.013087	-1.583629

E_{SCF}= -1168,000214 au
G_{423}= -1167,975307 au
E_{disp}= -21,7767 kcal·mol^{-1}

TS(1a-3a)

Ta	1.048405	-0.011601	-0.382370
O	-0.055263	1.498708	-0.179585
O	-0.077049	-1.500550	-0.152758
Si	-1.674166	1.554029	0.157677
Si	-1.706319	-1.531533	0.138681
O	-2.234192	0.015918	0.294376
O	-2.535399	2.231159	-1.061055
H	-2.295479	3.113461	-1.349150
O	-1.811825	2.380861	1.565754
H	-2.679688	2.451494	1.966902
O	-2.051239	-2.264373	1.563996
H	-1.899755	-3.208722	1.629399
O	-2.389971	-2.295494	-1.138770
H	-3.334803	-2.203793	-1.271740
C	3.144161	-0.002936	0.901181
H	2.887292	0.886188	1.481751
H	2.890821	-0.871717	1.512824
C	4.652431	-0.005638	0.578444
H	5.238726	0.013364	1.501459
H	4.937918	-0.898503	0.014123
H	4.933838	0.866542	-0.019299
H	2.026464	-0.027174	-1.848634
H	2.858023	-0.023040	-0.338947

E_{SCF}= -1246,566181 au
G_{423}= -1246,492907 au
E_{disp}= -27,9109 kcal·mol^{-1}

TS(1b-2)

Ta	-1.088281	-0.398844	-0.395404
O	-0.172430	1.283565	-0.243972
O	0.420552	-1.493897	-0.046060
Si	1.385132	1.734714	0.015633
Si	2.006435	-1.234264	0.316818
O	2.285216	0.380585	0.260141
O	1.547031	2.619106	1.390237
H	1.183460	3.506149	1.393485
O	1.871331	2.558963	-1.315524
H	2.810824	2.699517	-1.443780
O	3.010803	-1.907221	-0.788335
H	2.989752	-2.859316	-0.898348
O	2.227489	-1.837671	1.826587
H	3.060888	-1.661355	2.266614
C	-2.791689	0.686792	0.750254
C	-4.232989	0.308372	1.078948
H	-4.696930	-0.220532	0.242902
H	-4.288090	-0.345856	1.955903
H	-4.836211	1.194692	1.300145
H	-1.048212	-0.438786	-2.131761
H	-2.585452	-1.020309	-1.122659
H	-1.926325	-1.606060	0.802429
H	-2.781361	1.352982	-0.130856
H	-2.324595	1.242988	1.570379
H	-2.368537	-0.762515	0.891451

E_{SCF}= -1247,785447 au
G_{423}= -1247,695778 au
E_{disp}= -31,4889 kcal·mol^{-1}

2

Ta	1.121562	-0.207631	-0.454671
O	-0.229435	-1.455999	-0.064599
O	0.083808	1.399277	-0.224607
Si	-1.853756	-1.363907	0.250641
Si	-1.493611	1.672348	0.128729

O	-2.241424	0.221897	0.357954
O	-2.217602	-2.025968	1.703769
H	-2.165832	-2.979366	1.790414
O	-2.601868	-2.119101	-0.994597
H	-3.538261	-1.965350	-1.130569
O	-2.312278	2.379554	-1.105252
H	-1.972778	3.206008	-1.452904
O	-1.509328	2.571593	1.500020
H	-2.358014	2.783283	1.892384
C	2.476592	-0.142824	1.211185
H	1.877517	0.331143	2.007615
H	2.399196	-1.232545	1.409298
C	3.934106	0.288658	1.297682
H	4.529033	-0.182200	0.510789
H	4.032144	1.373383	1.186024
H	1.149182	0.135647	-2.175697
H	2.483873	-1.063667	-1.244304
H	2.354447	1.173875	-1.452936
H	2.699238	1.201321	-0.754282
H	4.385156	0.023990	2.260957

E_{SCF}= -1247,809276 au
G_{423}= -1247,721040 au
E_{disp}= -31,5317 kcal·mol^{-1}

3a

Ta	1.088087	-0.367589	-0.411510
O	-0.299432	-1.572777	-0.023984
O	0.312662	1.358576	-0.266080
Si	-1.902473	-1.266018	0.291720
Si	-1.251998	1.754165	0.083883
O	-2.095986	0.360316	0.320637
O	-2.330115	-1.799258	1.778376
H	-2.341987	-2.744645	1.937717
O	-2.740089	-1.981351	-0.916641
H	-3.668724	-1.770110	-1.026619
O	-1.997877	2.505633	-1.164794
H	-1.589812	3.292553	-1.530405
O	-1.192825	2.658520	1.446586
H	-2.016525	2.939639	1.848468
C	2.450280	-0.212858	1.242990
H	1.830881	0.198568	2.060163
H	2.675625	-1.253108	1.527031
C	3.743159	0.588222	1.102718
H	4.301025	0.631030	2.045596
H	4.396674	0.145239	0.346831
H	3.545321	1.622886	0.803050
H	1.261178	-0.171160	-2.144135
H	2.607531	-1.041504	-1.004288

E_{SCF}= -1246,628529 au
G_{423}= -1246,556156 au
E_{disp}= -29,2529 kcal·mol^{-1}

3b

Ta	1.185076	-0.414924	-0.222957
O	-0.356005	-1.455126	0.024092
O	0.303626	1.297722	-0.120119
Si	-1.985334	-1.180397	0.153113
Si	-1.257225	1.779737	0.004429
O	-2.201825	0.440123	0.179296
O	-2.575989	-1.751607	1.569573
H	-2.641428	-2.701579	1.680819
O	-2.671844	-1.893131	-1.151402
H	-3.562421	-1.638827	-1.398651
O	-1.817407	2.516395	-1.351320
H	-1.318617	3.258988	-1.696145
O	-1.340113	2.743110	1.329169
H	-2.197058	3.090015	1.582718
C	2.615105	-0.069854	1.311728
H	2.244835	0.486395	2.174150
H	3.131604	-0.975410	1.634579
C	3.403628	0.762319	0.317625
H	3.442900	1.820016	0.580333
H	4.404432	0.376248	0.125816
H	2.944405	0.762772	-0.726323
H	1.512151	0.038974	-1.874567
H	2.392389	-1.566564	-0.901900

E_{SCF}= -1246,631880 au
G_{423}= -1246,557070 au
E_{disp}= -29,8221 kcal·mol^{-1}

TS(3b-4)

Ta	-1.182916	-0.399855	-0.329892
O	-0.225762	1.271791	-0.246955
O	0.305578	-1.500478	0.031929
Si	1.326807	1.741994	-0.020240
Si	1.915472	-1.250404	0.281788
O	2.206679	0.359719	0.195429
O	1.366787	2.703980	1.302663
H	2.095899	3.321027	1.381857
O	1.956177	2.604706	-1.264307
H	2.229666	2.136259	-2.054871
O	2.828990	-1.930774	-0.898591
H	2.753260	-2.876664	-1.036219
O	2.242865	-1.858567	1.769002
H	3.129252	-1.751201	2.117979
C	-2.865339	1.239691	0.656708
H	-2.214251	1.989974	1.087065
H	-3.342947	1.475681	-0.291132
C	-3.239216	0.140803	1.360263
H	-2.896595	-0.013913	2.378459
H	-4.021538	-0.520971	1.012868
H	-2.068783	-1.375464	0.873612
H	-1.036615	-0.683130	-2.040477
H	-2.722039	-0.875347	-1.073658

E_{SCF}= -1246,580559 au
G_{423}= -1246,507590 au
E_{disp}= -30,0450 kcal·mol^{-1}

4

Ta	1.075889	-0.653912	-0.007056
O	0.469273	1.168275	0.004586
O	-0.588530	-1.511833	-0.029727
Si	-1.010072	1.886072	-0.008856

Si	-2.159306	-0.975785	-0.014250
O	-2.122527	0.659862	0.012611
O	-1.115002	2.788027	-1.364465
H	-1.711345	3.538218	-1.359992
O	-1.278156	2.869483	1.274493
H	-1.570879	2.479493	2.099890
O	-2.931763	-1.428568	1.357646
H	-3.067531	-2.364641	1.515651
O	-2.846329	-1.576803	-1.371241
H	-3.727041	-1.286426	-1.613743
C	3.370881	0.685778	0.729904
H	2.863128	1.479833	1.266346
H	3.931154	-0.028820	1.319866
C	3.416441	0.670971	-0.616656
H	2.946402	1.452023	-1.204745
H	4.015032	-0.055539	-1.151764
H	1.820713	-0.742433	-1.592947
H	1.699942	-0.708478	1.630488
H	2.402260	-1.848103	0.068293

E_{SCF}= -1246,589642 au
G_{423}= -1246,519770 au
E_{disp}= -30,2969 kcal·mol^{-1}

TS(3a-5)

Ta	1.196340	-0.149925	-0.319814
O	-0.187178	-1.412135	-0.002890
O	0.012574	1.357065	-0.131699
Si	-1.823384	-1.399294	0.190321
Si	-1.585118	1.624578	0.079365
O	-2.315194	0.160866	0.270273
O	-2.270769	-2.098685	1.604872
H	-2.178060	-3.049733	1.680586
O	-2.451062	-2.178016	-1.111683
H	-3.386902	-2.073031	-1.291690
O	-2.313401	2.300593	-1.229785
H	-1.992095	3.152845	-1.528855
O	-1.743134	2.555506	1.422077
H	-2.629648	2.749033	1.731218
C	2.708228	-0.333035	0.935455
H	2.774706	-1.058401	1.750403
H	2.675048	-1.297744	-0.402550
C	3.854418	0.655958	0.880626
H	4.815900	0.157116	0.713205
H	3.739813	1.400438	0.084067
H	3.921446	1.195958	1.831338
H	1.852715	0.532466	-1.823706
H	2.083611	-1.548125	-1.205960

E_{SCF}= -1246,592322 au
G_{423}= -1246,522956 au
E_{disp}= -29,3306 kcal·mol^{-1}

5

Ta	1.200093	-0.271730	-0.287699
O	-0.260406	-1.460534	-0.003695
O	0.157426	1.329513	-0.210448
Si	-1.885690	-1.299020	0.208201
Si	-1.421464	1.702921	0.008189
O	-2.251122	0.298124	0.221384
O	-2.380102	-1.892034	1.655283
H	-2.325213	-2.838963	1.793468
O	-2.585948	-2.078705	-1.055952
H	-3.520194	-1.932393	-1.213988
O	-2.095881	2.411728	-1.311031
H	-1.748596	3.260882	-1.589036
O	-1.508257	2.659956	1.338383
H	-2.376876	2.863812	1.689032
C	2.532424	-0.273677	1.107851
H	2.670373	-0.766879	2.068812
H	2.415993	-1.911253	-0.547058
C	3.457446	0.891153	0.807810
H	4.495813	0.571812	0.664324
H	3.187931	1.417692	-0.125690
H	3.427805	1.634730	1.613080
H	2.036446	0.082352	-1.821920
H	1.885016	-2.049358	-1.123840

E_{SCF}= -1246,597771 au
G_{423}= -1246,527001 au
E_{disp}= -29,6943 kcal·mol^{-1}

6

Ta	1.131966	-0.098405	-0.479284
O	0.145052	1.500740	-0.309574
O	-0.072878	-1.520775	-0.080384
Si	-1.458081	1.680624	0.075455
Si	-1.692059	-1.409635	0.218084
O	-2.108435	0.182704	0.224718
O	-2.291837	2.412411	-1.128114
H	-2.063116	3.315517	-1.354627
O	-1.490227	2.516341	1.482698
H	-2.320967	2.587000	1.955991
O	-2.084321	-1.964461	1.709919
H	-1.858404	-2.870829	1.926228
O	-2.440329	-2.227215	-0.986858
H	-3.398401	-2.222155	-1.019324
C	2.798904	-0.244949	0.422819
C	3.953435	0.289018	1.204704
H	2.773023	-1.363795	0.344892
H	4.907182	0.028503	0.730187
H	3.909456	1.379321	1.273365
H	1.741750	-0.314654	-2.118387
H	3.980316	-0.106738	2.227265

E_{SCF}= -1245,421102 au
G_{423}= -1245,366310 au
E_{disp}= -26,6029 kcal·mol^{-1}

TS(3a-7)

Ta	-1.247870	-0.098670	-0.273502
O	-0.043355	1.353891	0.017208
O	0.148944	-1.406108	-0.162061
Si	1.581027	1.583726	0.124838
Si	1.767744	-1.443116	0.075707
O	2.293271	0.110005	0.215689
O	1.992228	2.379609	1.498956
H	1.790193	3.315183	1.550088

O	2.036547	2.402400	-1.224174
H	2.967355	2.410469	-1.454034
O	2.588248	-2.065688	-1.203097
H	2.388265	-2.965578	-1.466387
O	2.026309	-2.293104	1.456058
H	2.919873	-2.329335	1.801393
H	-2.666006	0.975568	-0.847461
C	-3.313472	0.407410	0.594209
H	-3.493879	1.419828	0.953353
H	-4.196652	-0.029077	0.134517
C	-2.465932	-0.447390	1.429836
H	-2.717230	-1.510537	1.472428
H	-2.107193	-0.064434	2.383444
H	-1.952117	-0.994189	-1.642739
H	-1.976409	1.061612	-1.515675

E_{SCF}= -1246,610326 au
G_{423}= -1246,537280 au
E_{disp}= -29,8088 kcal·mol^{-1}

7

Ta	1.382726	0.096653	-0.562930
O	0.152256	-1.329203	-0.276684
O	0.055015	1.453834	-0.283522
Si	-1.461041	-1.500046	0.001436
Si	-1.531439	1.532571	0.103464
O	-2.101019	-0.008431	0.218912
O	-1.754941	-2.335108	1.382095
H	-1.570790	-3.275760	1.384127
O	-2.081807	-2.250636	-1.320952
H	-3.032502	-2.234011	-1.444317
O	-2.440202	2.242775	-1.065612
H	-2.239398	3.151214	-1.296859
O	-1.640083	2.319577	1.540076
H	-2.497919	2.361473	1.966058
H	2.648370	-1.123919	-1.392666
C	3.415076	-0.374027	0.287378
H	3.590289	-1.391444	0.635296
H	4.287029	0.047252	-0.207445
C	2.593410	0.489357	1.131374
H	2.828888	1.556710	1.154845
H	2.228455	0.119682	2.088498
H	1.968904	0.961859	-2.004408

E_{SCF}= -1246,611145 au
G_{423}= -1246,537260 au
E_{disp}= -29,8885 kcal·mol^{-1}

8

Ta	1.177306	-0.005432	-0.206790
O	0.081507	-1.533642	-0.060740
O	0.093259	1.534540	-0.098267
Si	-1.571833	-1.549558	0.070093
Si	-1.555128	1.564316	0.079824
O	-2.084424	0.009895	0.142860
O	-2.061365	-2.241146	1.470696
H	-1.873966	-3.171539	1.607033
O	-2.125130	-2.322072	-1.260705
H	-3.064681	-2.302397	-1.449993
O	-2.300659	2.234016	-1.213635
H	-2.076577	3.134720	-1.454153
O	-1.836743	2.363501	1.479065
H	-2.735388	2.413806	1.809206
H	1.670385	-0.018129	-1.886170
C	3.329514	-0.011633	-0.018959
H	3.842540	-0.916571	-0.344589
H	3.850151	0.882283	-0.362348
C	2.694330	0.004022	1.304914
H	2.751741	0.912527	1.906779
H	2.749157	-0.890990	1.926944

E_{SCF}= -1245,430704 au
G_{423}= -1245,373854 au
E_{disp}= -27,2908 kcal·mol^{-1}

TS(8-9)

Ta	1.147603	-0.001788	-0.019430
O	0.021260	-1.476901	0.105455
O	0.029213	1.469430	0.209778
Si	-1.633385	-1.553375	-0.016274
Si	-1.627631	1.552543	0.010651
O	-2.155388	0.006812	-0.131286
O	-2.170471	-2.310999	1.321281
H	-3.066409	-2.651328	1.323691
O	-2.143077	-2.403296	-1.318572
H	-2.048211	-2.009499	-2.187698
O	-1.965707	2.474172	-1.301752
H	-1.394376	2.378838	-2.066905
O	-2.377600	2.212015	1.297934
H	-2.389834	3.167508	1.372499
H	2.476613	0.026164	-1.347105
C	3.493905	-0.020631	-0.554762
H	3.962699	-0.919311	-0.956974
H	4.005771	0.869013	-0.922974
C	3.120031	-0.042387	0.875944
H	3.383020	0.837753	1.462254
H	3.360438	-0.948760	1.430544

E_{SCF}= -1245,390487 au
G_{423}= -1245,331756 au
E_{disp}= -26,9235 kcal·mol^{-1}

TS(3a-9)

Ta	1.077826	-0.080080	0.053739
O	-0.145531	-1.505521	0.030322
O	0.070620	1.483938	0.006268
Si	-1.798773	-1.426524	0.045678
Si	-1.581288	1.648861	0.029026
O	-2.251503	0.152303	0.005676
O	-2.430017	-2.029186	1.433201
H	-2.249936	-2.945487	1.649903
O	-2.300091	-2.242920	-1.282064
H	-3.230647	-2.212864	-1.510249
O	-2.128733	2.404801	-1.315629
H	-1.843196	3.305626	-1.476697
O	-1.928476	2.466444	1.404021
H	-2.837841	2.487073	1.706417
C	3.091473	-0.000174	0.799105

H	3.055366	0.784363	1.572320
H	3.341790	-0.925079	1.339800
C	4.184767	0.340750	-0.232798
H	5.153586	0.489817	0.257182
H	4.314739	-0.452543	-0.973928
H	3.963321	1.260221	-0.785028
H	2.152211	-1.749933	-1.378185
H	2.480192	-2.230013	-0.887842

E_{SCF}= -1246,566172 au
G_{423}= -1246,498301 au
E_{disp}= -28,3003 kcal·mol^{-1}

9

Ta	1.096047	-0.133665	-0.152967
O	0.158950	1.484981	-0.132548
O	-0.155895	-1.513883	0.005762
Si	-1.481632	1.700440	-0.013860
Si	-1.808500	-1.371415	0.071810
O	-2.197077	0.223029	0.028280
O	-2.093842	2.453202	-1.332505
H	-1.796443	3.344431	-1.522922
O	-1.724623	2.543551	1.368338
H	-2.616401	2.605298	1.714491
O	-2.405891	-1.935174	1.489153
H	-2.258055	-2.857299	1.705898
O	-2.382429	-2.184965	-1.226786
H	-3.314273	-2.110007	-1.438804
C	3.103459	-0.448499	0.129923
H	3.243639	-1.489996	0.458983
H	2.985203	-0.537997	-1.027491
C	4.283503	0.444175	0.470560
H	5.225638	0.073798	0.051702
H	4.139009	1.465364	0.106335
H	4.400593	0.500618	1.555463

E_{SCF}= -1245,395130 au
G_{423}= -1245,338509 au
E_{disp}= -25,9591 kcal·mol^{-1}

TS(9-6)

Ta	1.099338	-0.104226	-0.144820
O	0.130576	1.512513	-0.088694
O	-0.124752	-1.532399	-0.007452
Si	-1.512769	1.678342	0.030291
Si	-1.776001	-1.412720	0.050931
O	-2.183785	0.178727	0.041848
O	-2.150970	2.436630	-1.274135
H	-1.871758	3.336043	-1.453378
O	-1.786552	2.484486	1.429623
H	-2.687655	2.544970	1.751123
O	-2.380538	-2.014194	1.450629
H	-2.218357	-2.937780	1.650229
O	-2.336904	-2.198620	-1.271436
H	-3.271979	-2.139758	-1.474317
C	3.011961	-0.372215	0.214057
C	4.316315	0.356853	0.357549
H	3.111296	-1.469067	0.326957
H	5.091439	-0.039357	-0.308331
H	4.209644	1.426583	0.160512
H	2.549964	-0.324846	-1.237292
H	4.680488	0.247998	1.383998

E_{SCF}= -1245,388694 au
G_{423}= -1245,333715 au
E_{disp}= -26,4517 kcal·mol^{-1}

TS(9-10)

Ta	1.139163	-0.005100	-0.041308
O	0.016129	-1.510704	0.058081
O	0.044879	1.526424	-0.065641
Si	-1.638299	-1.521550	0.123962
Si	-1.605748	1.571996	0.045185
O	-2.170041	0.032629	0.156415
O	-2.187619	-2.206338	1.508421
H	-2.024123	-3.141846	1.639244
O	-2.145718	-2.320616	-1.213294
H	-3.069102	-2.250131	-1.460807
O	-2.295934	2.196947	-1.304180
H	-2.016433	3.068020	-1.590779
O	-1.945798	2.444594	1.389532
H	-2.862820	2.524412	1.657412
C	3.015278	-0.050650	-0.677639
H	3.586134	0.831721	-0.972965
H	3.561591	-0.967704	-0.906491
C	3.180940	0.021535	1.280448
H	2.960195	-0.840864	1.912353
H	4.253645	0.001567	1.067840
H	2.978976	0.934589	1.843781

E_{SCF}= -1245,363009 au
G_{423}= -1245,306145 au
E_{disp}= -26,8928 kcal·mol^{-1}

TS(8-10)

Ta	1.276249	-0.088044	-0.083737
O	-0.094194	-1.489988	0.023125
O	0.124786	1.405602	-0.075066
Si	-1.717112	-1.455155	-0.025245
Si	-1.518704	1.597337	0.016737
O	-2.215322	0.123604	-0.056042
O	-2.423190	-2.079452	1.324925
H	-2.166337	-2.966600	1.581989
O	-2.204949	-2.237274	-1.385859
H	-3.146645	-2.278124	-1.560869
O	-2.084885	2.454656	-1.259963
H	-1.887883	3.392135	-1.292851
O	-1.798058	2.351943	1.447948
H	-2.680770	2.299618	1.818614
C	3.147741	0.256869	-0.747670
H	3.460642	1.210860	-1.191777
H	1.811072	-0.576492	-1.750550
C	2.362191	-0.265901	1.587804
H	3.385534	-0.578485	1.784624
H	1.916772	0.238408	2.456568
H	3.949741	-0.483211	-0.807200

E_{SCF}= -1245,340079 au
G_{423}= -1245,288930 au

E_{disp}= -27,9736 kcal·mol^{-1}

10

Ta	1.359181	0.005239	-0.147548
O	0.242891	1.528941	-0.080875
O	0.240803	-1.518214	-0.010749
Si	-1.407768	1.563408	0.052164
Si	-1.411504	-1.542838	0.061470
O	-1.946627	0.011701	0.053846
O	-2.106281	2.272320	-1.248491
H	-1.938784	3.204218	-1.399546
O	-1.734774	2.335085	1.457457
H	-2.630654	2.312354	1.797898
O	-1.959720	-2.190612	1.461909
H	-1.689083	-3.082569	1.686550
O	-1.908110	-2.361463	-1.266330
H	-2.848469	-2.425462	-1.441611
C	2.810861	0.021511	1.107819
H	3.239135	-0.910115	1.492069
H	3.228983	0.909018	1.589107
C	2.368814	-0.056037	-2.049841
H	3.004792	0.825357	-2.193028
H	3.027823	-0.927527	-2.134190
H	1.642815	-0.094289	-2.874190

E_{SCF}= -1245,432945 au

G_{423}= -1245,380544 au

E_{disp}= -27,2676 kcal·mol^{-1}

III. Reaction of Ta-alkylidene 10 with ethane

TS(3a-10)

Ta	1.059381	-0.039663	-0.358529
O	0.174801	-1.741524	-0.146514
O	0.259028	1.714070	-0.271844
Si	-1.433119	-1.570167	0.176669
Si	-1.335164	1.646217	0.143567
O	-1.734495	0.050059	0.284031
O	-1.863962	-2.180920	1.637731
H	-1.780415	-3.127169	1.767586
O	-2.257144	-2.261486	-1.060289
H	-3.207623	-2.141939	-1.098007
O	-2.336626	2.240545	-1.012569
H	-2.218860	3.153015	-1.282316
O	-1.491622	2.429161	1.575330
H	-2.350633	2.431845	2.001125
C	2.968553	-0.066510	0.156324
H	3.584091	0.825064	0.285147
H	3.540965	-0.975140	0.349372
C	1.881735	0.024858	1.883694
H	1.343315	-0.849604	2.260930
H	2.868548	0.019043	2.347236
H	1.387179	0.951747	2.188654
H	0.004378	-0.078550	-2.038503
H	0.852744	-0.104413	-2.239192
O	3.038858	-1.947480	-0.970266
H	2.922111	-2.881956	-1.148789
O	2.378303	-1.973316	1.674014
H	3.257134	-1.898334	2.050026
C	-2.638398	1.028110	0.800891
H	-2.399563	1.748795	0.000686
H	-2.231636	1.448040	1.728398
H	-2.390371	-0.403648	0.893254
C	-1.808522	-0.376784	-2.007038
H	-1.888349	-1.353461	-2.495169
C	-4.155117	0.871445	0.877741
H	-4.451994	0.186314	1.678818
H	-4.646130	1.829103	1.078560
H	-4.550032	0.475901	-0.061760
H	-2.075134	0.446191	-2.674798
C	-2.098681	-1.783724	1.001983
H	-1.443731	-2.013451	1.845394
H	-3.138225	-1.921423	1.312319
H	-1.922137	-2.513555	0.202274

E_{SCF}= -1246,529721 au

G_{423}= -1246,457045 au

E_{disp}= -32,0870 kcal·mol^{-1}

E_{SCF}= -1325,206898 au

G_{423}= -1325,087933 au

E_{disp}= -38,6249 kcal·mol^{-1}

TS(10-11)

Ta	-0.966764	-0.184881	-0.289500
O	0.112481	1.392171	-0.159444
O	0.510347	-1.408044	-0.088259
Si	1.706060	1.730717	0.041088
Si	2.112623	-1.275462	0.208197
O	2.519079	0.317900	0.226440
O	1.984215	2.587366	1.416009
H	1.708039	3.505189	1.428071
O	2.190027	2.549770	-1.296958
H	3.129736	2.591502	-1.481444

11

Ta	0.938098	-0.032468	0.018104
O	-0.257331	-1.450503	0.398489
O	-0.102777	1.495115	-0.422269
Si	-1.912460	-1.398296	0.360292
Si	-1.750372	1.610000	-0.405249
O	-2.363141	0.139954	0.005004
O	-2.561014	-1.720729	1.829694
H	-2.437291	-2.598641	2.194732
O	-2.376214	-2.462893	-0.792964
H	-3.289730	-2.456957	-1.083641
O	-2.365609	1.941299	-1.886696
H	-2.061374	2.730475	-2.338234
O	-2.115009	2.749259	0.713203
H	-3.037448	2.912272	0.917228
C	2.309430	-0.427054	-1.266852

H	2.766061	0.424895	-1.785991
C	2.070781	0.427949	1.787908
H	2.358741	-0.565039	2.173338
H	1.351044	0.827974	2.522656
C	3.304848	1.330304	1.714899
H	3.751405	1.492520	2.703509
H	4.065225	0.891777	1.064249
H	3.058456	2.318087	1.311449
H	2.649861	-1.388619	-1.654552

E_{SCF}= -1284,738886 au
G_{423}= -1284,660847 au
E_{disp}= -31,0762 kcal·mol^{-1}

TS(11-13)

Ta	1.110338	-0.041516	-0.188079
O	-0.145155	-1.437018	0.060734
O	-0.142155	1.440473	-0.181442
Si	-1.790648	-1.497109	0.201559
Si	-1.748020	1.560186	0.078199
O	-2.359299	0.035624	0.240989
O	-2.252880	-2.191619	1.613796
H	-2.063024	-3.123388	1.735729
O	-2.320430	-2.331643	-1.108273
H	-3.260226	-2.325432	-1.297996
O	-2.562125	2.206381	-1.195280
H	-2.299317	3.079219	-1.492001
O	-1.964090	2.430937	1.453763
H	-2.860574	2.550251	1.771960
C	2.388636	-0.282325	-1.677317
H	3.214748	0.408238	-1.868384
C	2.470293	-0.025685	1.249680
H	2.809107	-0.720081	-0.140765
H	1.958725	-0.497843	2.107738
C	3.873711	0.410350	1.577428
H	4.475069	-0.401106	2.006713
H	4.400942	0.784330	0.693811
H	3.859339	1.222992	2.312615
H	2.384859	-1.119464	-2.378712

E_{SCF}= -1284,684238 au
G_{423}= -1284,608731 au
E_{disp}= -31,4296 kcal·mol^{-1}

13

Ta	1.274864	-0.239376	0.113364
O	-0.016480	-1.599811	0.318965
O	0.147146	1.298791	-0.110417
Si	-1.670844	-1.586874	0.245987
Si	-1.484084	1.458312	-0.104840
O	-2.159447	-0.031571	0.099061
O	-2.335958	-2.141760	1.636955
H	-2.215464	-3.067510	1.854994
O	-2.072954	-2.497524	-1.055957
H	-2.971476	-2.448035	-1.386648
O	-2.075836	1.996528	-1.538828
H	-1.709244	2.807820	-1.894665
O	-1.854025	2.457224	1.142439
H	-2.778126	2.654311	1.304389
C	2.473991	-0.424074	-1.341660
H	2.949863	0.541295	-1.004543
C	2.510652	0.074915	1.853795
H	3.026779	-0.869155	2.080249
H	3.290414	0.835834	1.746109
H	1.895362	0.337772	2.724467
C	3.039703	-0.993040	-2.599439
H	2.946744	-0.303292	-3.447505
H	4.103753	-1.238352	-2.493698
H	2.518881	-1.915905	-2.869393

E_{SCF}= -1284,744961 au
G_{423}= -1284,667774 au
E_{disp}= -30,3793 kcal·mol^{-1}

TS(10-12a)

Ta	-0.979178	-0.536121	-0.114770
O	-0.157225	1.184270	0.012177
O	0.767100	-1.361056	-0.178632
Si	1.336275	1.864513	0.067409
Si	2.342509	-0.973610	-0.003427
O	2.452811	0.666792	0.077851
O	1.581863	2.715552	1.451489
H	1.081380	3.524313	1.570632
O	1.450223	2.819155	-1.264849
H	2.310885	3.178053	-1.487432
O	3.262537	-1.404426	-1.295306
H	3.301768	-2.335294	-1.520574
O	2.866071	-1.683286	1.384084
H	3.761305	-1.497547	1.672609
C	-2.881754	0.714563	0.725621
H	-2.320802	0.846934	1.658973
H	-3.783521	0.160058	1.005314
H	-2.737820	-0.028669	-0.524923
C	-2.107816	-0.803282	-1.698117
H	-2.632585	-1.767512	-1.721924
C	-3.232476	2.078956	0.134882
H	-3.836285	1.978446	-0.774106
H	-3.805158	2.688599	0.841390
H	-2.329430	2.633267	-0.131809
H	-2.276903	-0.210226	-2.595183
C	-1.583059	-1.931008	1.414661
H	-1.275506	-2.930664	1.075389
H	-1.062858	-1.747020	2.362286
H	-2.659138	-1.947402	1.613597

E_{SCF}= -1325,224132 au
G_{423}= -1325,105885 au
E_{disp}= -38,8759 kcal·mol^{-1}

12a

Ta	-1.331197	0.422212	0.027207
O	0.189715	1.646573	0.084714
O	-0.245372	-1.111464	-0.056908
Si	1.813637	1.522807	-0.001175
Si	1.366467	-1.482744	-0.021828
O	2.204302	-0.080810	-0.050754
O	2.581118	2.099961	1.332983
H	2.488276	3.034219	1.527024

O	2.292887	2.286759	-1.374236
H	3.209539	2.198381	-1.641028
O	1.821401	-2.325107	-1.351457
H	1.497089	-3.221881	-1.449783
O	1.592603	-2.327913	1.365566
H	2.490393	-2.473277	1.668992
C	-1.946990	1.238899	1.917654
H	-2.613713	0.825081	-2.402565
H	-2.464792	2.185200	1.698740
H	-1.089989	1.475545	2.556059
H	-2.642084	0.599179	2.468117
C	-1.932904	1.412857	-1.781196
H	-1.071809	1.728310	-2.378113
H	-2.466913	2.324094	-1.470543
C	-3.294875	-0.528305	-0.031497
H	-3.237773	-1.160716	-0.937733
H	-3.235774	-1.247667	0.807890
C	-4.638535	0.196544	0.005303
H	-4.743179	0.880311	-0.843443
H	-5.492502	-0.490178	-0.027147
H	-4.741651	0.795253	0.916350

E_{SCF}= -1325,273792 au
G_{423}= -1325,153903 au
E_{disp}= -38,2868 kcal·mol^{-1}

12b

Ta	-1.17057	0.02123	-0.17296
O	0.21057	-1.31902	-0.10901
O	0.21629	1.31300	0.16654
Si	1.83424	-1.50324	-0.04126
Si	1.84332	1.48860	0.12348
O	2.50823	-0.01255	0.10172
O	2.47775	-2.14183	-1.41303
H	2.20451	-3.02644	-1.66174
O	2.13326	-2.44599	1.27109
H	3.04845	-2.59656	1.51355
O	2.42304	2.22387	1.47253
H	2.24878	3.16091	1.57431
O	2.20818	2.33410	-1.23896
H	3.12210	2.34607	-1.52870
C	-2.04096	-1.26296	-1.69460
H	-1.51853	-1.19749	-2.65568
H	-3.09575	-1.02859	-1.88251
H	-3.09461	-0.98303	1.27016
C	-2.43097	-0.13571	1.51728
H	-3.06888	0.76366	1.45729
C	-1.99966	1.57715	-1.43710
H	-1.95444	2.52492	-0.88289
H	-1.41803	1.72077	-2.35470
H	-3.03821	1.38573	-1.73036
C	-1.83938	-0.29654	2.92157
H	-1.19651	0.54844	3.18189
H	-2.62544	-0.35928	3.68145
H	-1.23445	-1.20378	2.99703
H	-1.96578	-2.30468	-1.35416

E_{SCF}= -1325,276252 au
G_{423}= -1325,156785 au
E_{disp}= -37,8542 kcal·mol^{-1}

TS(12b-13)

Ta	-0.939403	-0.432951	-0.165464
O	-0.095461	1.264071	0.139318
O	0.800152	-1.270535	-0.268380
Si	1.403010	1.915273	0.254156
Si	2.375584	-0.916937	-0.027606
O	2.511222	0.708498	0.186383
O	1.652760	2.663023	1.697061
H	1.128530	3.443114	1.885427
O	1.548858	2.960683	-1.006844
H	2.416686	3.328803	-1.181443
O	3.316133	-1.260715	-1.332168
H	3.363286	-2.176385	-1.611610
O	2.861248	-1.745548	1.307693
H	3.744526	-1.576406	1.640014
C	-2.833608	0.815831	0.630929
H	-2.420154	0.844003	1.644032
H	-3.872849	0.488004	0.726607
H	-2.704461	0.008228	-0.574683
C	-2.037921	-0.729771	-1.742158
H	-2.195598	-1.806017	-1.483713
C	-1.587330	-1.885140	1.307065
H	-1.254381	-2.884588	0.997788
H	-1.109181	-1.677595	2.272565
H	-2.669911	-1.916157	1.463073
C	-2.645056	-0.304456	-3.041991
H	-2.166994	-0.823871	-3.879644
H	-3.718822	-0.520907	-3.095870
H	-2.509086	0.767754	-3.204838
H	-2.813182	1.833395	0.233746

E_{SCF}= -1325,229394 au
G_{423}= -1325,111125 au
E_{disp}= -38,1302 kcal·mol^{-1}

TS(13-14)

Ta	1.005207	-0.146124	0.280394
O	-0.112425	1.386330	0.091520
O	-0.487463	-1.408218	0.176017
Si	-1.715689	1.700821	-0.103352
Si	-2.077237	-1.309344	-0.142379
O	-2.514563	0.278958	-0.233284
O	-2.007797	2.516408	-1.499902
H	-1.737219	3.435144	-1.538805
O	-2.184212	2.562188	1.214746
H	-3.120044	2.588707	1.420681
O	-3.025385	-1.936533	1.047928
H	-2.877467	-2.852167	1.289566
O	-2.335248	-2.066416	-1.582771
H	-3.224510	-2.041662	-1.940505
C	2.696763	0.996354	-0.833832
H	2.415182	1.753139	-0.080192
H	2.347357	1.377318	-1.801545
H	2.389801	-0.440074	-0.938202
C	1.872190	-0.311263	1.963308
H	1.950806	-1.422810	1.834650

C	4.212716	0.830109	-0.816595
H	4.546011	0.085554	-1.547774
H	4.725701	1.766523	-1.060171
H	4.552035	0.500627	0.168749
C	2.030832	-1.781323	-1.103492
H	1.320278	-1.916605	-1.921790
H	3.042857	-1.937098	-1.490113
H	1.860760	-2.564729	-0.358772
C	2.289130	0.186558	3.307878
H	1.708172	-0.271406	4.117901
H	3.346586	-0.027563	3.507534
H	2.155168	1.269316	3.380205

E_{SCF}= -1364,518328 au
G_{423}= -1364,375974 au
E_{disp}= -42,2285 kcal·mol^{-1}

14

Ta	0.96216	-0.10356	0.03002
O	-0.31079	-1.44186	0.44847
O	-0.11722	1.40412	-0.46181
Si	-1.96370	-1.39892	0.38816
Si	-1.75127	1.56768	-0.43130
O	-2.42082	0.12868	0.01018
O	-2.62846	-1.71521	1.85260
H	-2.50838	-2.59242	2.22034
O	-2.40579	-2.48471	-0.75696
H	-3.31222	-2.47459	-1.06906
O	-2.37912	1.89318	-1.91233
H	-2.03810	2.65573	-2.38287
O	-2.08228	2.74046	0.66666
H	-3.00147	2.94524	0.84626
C	2.28078	-0.49456	-1.28066
H	2.59146	0.58636	-1.25362
C	2.10192	0.44268	1.77234
H	2.34919	-0.54912	2.19379
H	1.38453	0.88555	2.48355
C	2.98963	-1.31630	-2.30605
H	2.84199	-0.93125	-3.32277
H	4.07126	-1.34832	-2.12504
H	2.62758	-2.34814	-2.29162
C	3.36656	1.30010	1.69900
H	3.80805	1.46837	2.68881
H	4.12376	0.82463	1.07003
H	3.15662	2.28631	1.27224

E_{SCF}= -1324,050661 au
G_{423}= -1323,948244 au
E_{disp}= -34,2954 kcal·mol^{-1}

TS(14-6)

Ta	1.04984	-0.18084	-0.14479
O	-0.10987	1.34551	0.07359
O	-0.40693	-1.45294	-0.15555
Si	-1.71218	1.60150	0.28886
Si	-2.03511	-1.38109	-0.15610
O	-2.50173	0.17562	0.10837
O	-2.33960	2.60395	-0.85570
H	-2.11540	3.53367	-0.79236
O	-1.90088	2.22524	1.79916
H	-2.78140	2.20956	2.17790
O	-2.71407	-2.24231	1.07032
H	-2.50055	-3.17544	1.12045
O	-2.54651	-1.91124	-1.62779
H	-3.48791	-1.87605	-1.80610
C	2.23012	-0.60696	1.27582
H	2.23620	-1.64778	0.82914
C	2.37168	1.43354	-1.36334
H	2.80831	1.84319	-0.45503
H	1.67528	2.05866	-1.91035
C	2.93038	-0.49052	2.58559
H	2.50959	-1.16280	3.34335
H	3.99819	-0.72765	2.49788
H	2.85263	0.52931	2.97245
C	2.90034	0.30443	-1.92998
H	2.66306	0.02928	-2.95151
H	3.75138	-0.20210	-1.49066
H	1.77615	-1.08967	-1.53186

E_{SCF}= -1324,001469 au
G_{423}= -1323,899366 au
E_{disp}= -35,3370 kcal·mol^{-1}

TS(13-15)

Ta	0.894272	-0.462619	-0.143840
O	-0.023340	1.221866	-0.102185
O	-0.800147	-1.373638	0.091187
Si	-1.535516	1.821901	0.099370
Si	-2.399423	-1.058343	0.123990
O	-2.597374	0.575363	0.160141
O	-2.015134	2.750572	-1.169696
H	-1.551577	3.577359	-1.312185
O	-1.502246	2.680068	1.502082
H	-2.338649	2.986687	1.856473
O	-3.138959	-1.611884	1.484963
H	-3.126874	-2.558088	1.637730
O	-3.057128	-1.715092	-1.233498
H	-3.984314	-1.543018	-1.406593
C	2.627035	0.925578	-1.102546
H	1.968245	1.093026	-1.963379
H	3.523031	0.448999	-1.514585
H	2.671327	0.029490	0.079340
C	2.211355	-0.862066	1.230880
H	2.421083	-1.876194	0.808555
C	2.969196	2.262455	-0.445740
H	3.679774	2.137794	0.378660
H	3.422449	2.956979	-1.161101
H	2.074561	2.739651	-0.038855
C	2.936300	-0.561371	2.505965
H	2.615351	-1.246242	3.298438
H	4.023454	-0.664919	2.407993
H	2.723621	0.454517	2.847328
C	1.348916	-1.725502	-1.845940
H	2.392219	-1.696745	-2.174131
H	1.095849	-2.763780	-1.592737
H	0.715514	-1.446746	-2.697327

E_{SCF}= -1364,535779 au

G_{423}= -1364,391540 au
E_{disp}= -42,699900 kcal·mol^{-1}

15

Ta	1.203196	-0.296109	-0.260983
O	0.246172	1.318806	0.149748
O	-0.455586	-1.228107	0.056484
Si	-1.247509	1.893274	0.491908
Si	-2.065835	-0.969845	0.177370
O	-2.296539	0.630765	0.468482
O	-1.814443	2.952174	-0.630408
H	-1.372455	3.799211	-0.707554
O	-1.139675	2.583835	1.980050
H	-1.952517	2.876103	2.396005
O	-2.729549	-1.761162	1.454519
H	-2.801370	-2.715083	1.394094
O	-2.746223	-1.429614	-1.247724
H	-3.649522	-1.159449	-1.422140
C	2.330653	0.917285	-1.678637
H	1.910973	0.854660	-2.689663
H	3.282657	0.357669	-1.738921
H	3.380556	0.000995	1.170032
C	2.581416	-0.751393	1.282356
H	3.032952	-1.708276	0.966188
C	2.611969	2.374585	-1.302841
H	3.025506	2.475739	-0.293280
H	3.328852	2.839466	-1.990694
H	1.693440	2.965703	-1.326396
C	2.104802	-0.824740	2.737269
H	1.334878	-1.589904	2.866538
H	2.928946	-1.067531	3.416428
H	1.678460	0.127294	3.064422
C	1.447020	-1.783973	-1.824505
H	2.428079	-1.780264	-2.310859
H	1.288355	-2.766205	-1.355159
H	0.682209	-1.688851	-2.603372

E_{SCF}= -1364,580908 au
G_{423}= -1364,436384 au
E_{disp}= -42,424600 kcal·mol^{-1}

TS(15-14)

Ta	0.944500	-0.031239	0.047318
O	-0.391766	1.312590	-0.293370
O	-0.463046	-1.315460	0.383873
Si	-2.017960	1.489168	-0.308694
Si	-2.087213	-1.454219	0.288877
O	-2.716595	0.030426	-0.032023
O	-2.583527	1.973819	-1.775320
H	-2.325880	2.845234	-2.080405
O	-2.378516	2.577466	0.870893
H	-3.302086	2.692689	1.100774
O	-2.773859	-1.916830	1.709842
H	-2.529389	-2.775264	2.059177
O	-2.409910	-2.523060	-0.919548
H	-3.325589	-2.637302	-1.179733
C	2.299036	1.688863	-0.945434
H	1.863612	1.515487	-1.934717
H	3.381886	1.755237	-1.083637
H	2.539282	0.914446	0.259859
C	2.221489	0.097349	1.507645
H	2.609149	-0.926938	1.275938
C	2.835583	0.740358	2.710309
H	2.579039	0.185465	3.619328
H	3.929908	0.783625	2.653231
H	2.465061	1.760752	2.838450
C	1.826838	-1.376604	-1.412833
H	1.679435	-2.360815	-0.938942
H	1.128234	-1.380533	-2.264269
C	3.266738	-1.258383	-1.914688
H	3.988618	-1.270236	-1.091354
H	3.525609	-2.087557	-2.583723
H	3.429339	-0.332777	-2.472509
H	1.927349	2.648529	-0.579031

E_{SCF}= -1364,533373 au
G_{423}= -1364,389457 au
E_{disp}= -42,619100 kcal·mol^{-1}

IV. Reaction of Ta-alkyl 3a with ethane

TS(3a-16)

Ta	0.974099	-0.413626	0.024552
O	0.083989	1.297754	0.009301
O	-0.603151	-1.484556	-0.074805
Si	-1.485210	1.770013	-0.020297
Si	-2.210836	-1.184109	-0.217495
O	-2.443265	0.437477	-0.120964
O	-1.844732	2.661934	-1.353238
H	-1.429105	3.521930	-1.435439
O	-1.749978	2.600061	1.371486
H	-2.656190	2.810003	1.603495
O	-3.073451	-1.834254	1.017055
H	-3.088120	-2.789347	1.098299
O	-2.664604	-1.777704	-1.679669
H	-3.538589	-1.555746	-2.005435
C	2.375909	0.671903	-1.498045
C	3.695338	0.263750	-2.146889
H	4.333838	-0.262948	-1.433476
H	3.536804	-0.403155	-3.001616
H	4.243881	1.135937	-2.517419
H	2.615923	-1.034923	0.304078
H	1.481723	-1.602465	-1.369791
H	2.579518	1.352252	-0.654533
H	1.736867	1.223837	-2.195748
H	1.889014	-0.765327	-1.554425
C	1.259329	-0.494583	2.154256
H	1.433995	-1.540868	2.435517
H	0.266904	-0.223193	2.551166
C	2.330785	0.411324	2.762169
H	2.319911	0.364993	3.857440

H	3.329962	0.120875	2.426512
H	2.177568	1.460263	2.487942

E_{SCF}= -1326,414445 au
G_{423}= -1326,274630 au
E_{disp}= -40,2863 kcal·mol^{-1}

TS(6-16)

Ta	0.900039	-0.469911	-0.275904
O	0.021910	1.195685	0.082989
O	-0.759970	-1.443512	-0.159054
Si	-1.500752	1.737054	0.372305
Si	-2.361662	-1.124834	-0.087076
O	-2.543513	0.482711	0.214387
O	-1.985193	2.856438	-0.728642
H	-1.529686	3.699790	-0.733861
O	-1.486409	2.346260	1.898850
H	-2.328169	2.576229	2.295972
O	-3.100895	-1.885957	1.168391
H	-3.100037	-2.844540	1.164988
O	-3.017447	-1.547041	-1.532886
H	-3.937119	-1.326110	-1.689479
C	2.572879	0.919292	-1.266188
H	1.189767	-1.222524	-1.846606
H	1.818600	1.231234	-1.999683
H	3.377548	0.478665	-1.863021
H	2.723640	-0.174116	-0.277252
C	2.333596	-1.169146	0.823443
H	2.248854	-2.123699	0.232386
C	3.327196	-1.212589	1.937559
H	4.337165	-1.459361	1.589795
H	3.374354	-0.249576	2.451899
H	3.043914	-1.967215	2.679030
C	3.066731	2.128943	-0.470931
H	3.865277	1.854887	0.226876
H	3.467164	2.904709	-1.132157
H	2.258028	2.575414	0.112905

E_{SCF}= -1325,213416 au
G_{423}= -1325,092427 au
E_{disp}= -37,2312 kcal·mol^{-1}

TS(8-16)

Ta	1.146183	-0.095460	-0.205493
O	-0.197001	-1.382753	0.051359
O	-0.274684	1.315639	-0.082474
Si	-1.807357	-1.589261	0.347878
Si	-1.883373	1.400663	-0.091434
O	-2.492969	-0.108613	0.213633
O	-1.920401	-2.231895	1.848036
H	-2.711595	-2.730273	2.057890
O	-2.528295	-2.636514	-0.690061
H	-2.839414	-2.286997	-1.527194
O	-2.551561	1.806855	-1.548180
H	-2.211785	2.594177	-1.976572
O	-2.351973	2.460399	1.081377
H	-3.289839	2.647434	1.148264
C	2.431324	-1.572446	-1.206082
H	2.993683	-1.221932	-2.066471
C	1.982573	1.003733	1.627410
H	1.035164	1.317253	2.066403
H	2.685513	0.794913	2.438646
H	1.900525	-2.503034	-1.394691
C	2.555457	2.001603	0.625681
H	2.084551	2.979727	0.710307
H	3.639189	2.092997	0.707172
H	2.386112	1.736819	-0.459791
C	3.023248	-1.379922	0.108348
H	2.943171	-2.178359	0.846660
H	3.998545	-0.893161	0.150566
H	2.335042	-0.234789	1.162674
H	1.381880	0.633728	-1.783507

E_{SCF}= -1325,216133 au
G_{423}= -1325,091827 au
E_{disp}= -39,8648 kcal·mol^{-1}

16

Ta	1.202488	-0.239645	-0.432725
O	0.265632	1.293218	0.196832
O	-0.385348	-1.297317	-0.160545
Si	-1.244717	1.755787	0.649301
Si	-1.994845	-1.101696	0.051745
O	-2.239196	0.461720	0.503364
O	-1.876115	2.914724	-0.327102
H	-1.456444	3.776526	-0.330123
O	-1.108100	2.266394	2.204494
H	-1.914013	2.466479	2.683688
O	-2.574288	-2.020707	1.283392
H	-2.641100	-2.965585	1.136509
O	-2.742327	-1.441671	-1.370654
H	-3.656355	-1.172108	-1.475883
C	2.346841	1.016096	-1.777770
H	1.160039	-1.076348	-1.975671
H	1.791401	1.269035	-2.687896
H	3.162769	0.357595	-2.125762
H	3.557616	-0.404215	0.787297
C	2.686399	-1.077337	0.815478
H	2.961674	-1.937158	0.166403
C	2.395504	-1.546848	2.242365
H	3.260860	-2.050705	2.685717
H	2.141605	-0.702762	2.889376
H	1.555211	-2.245181	2.269510
C	2.924105	2.280378	-1.122936
H	3.471723	2.068532	-0.196497
H	3.627421	2.795790	-1.788318
H	2.130218	2.985976	-0.864962

E_{SCF}= -1325,258881 au
G_{423}= -1325,137969 au
E_{disp}= -37,7301 kcal·mol^{-1}

TS(16-17)

Ta	1.00711	-0.33454	-0.12987
O	-0.56687	-1.42028	-0.21412
O	-0.07354	1.23000	0.23863
Si	-2.19698	-1.24726	-0.21677
Si	-1.63604	1.64049	0.45379

O	-2.55406	0.29924	0.19386
O	-2.91985	-2.19683	0.91186
H	-2.91383	-3.14346	0.76139
O	-2.70969	-1.60813	-1.73722
H	-3.60675	-1.36655	-1.97440
O	-2.17347	2.75063	-0.63557
H	-1.81735	3.63833	-0.57363
O	-1.79187	2.18786	1.99682
H	-2.67933	2.33838	2.32673
C	2.18372	-1.03105	1.29938
H	1.68092	-1.74726	1.96338
H	2.15565	-1.82325	-0.14974
C	3.60484	-0.73290	1.70835
H	4.21065	-1.64413	1.78153
H	4.11016	-0.05271	1.01736
H	3.61471	-0.26208	2.69810
H	1.74913	-1.78974	-1.08517
C	2.17502	0.70812	-1.62208
H	3.07994	0.10228	-1.78918
H	1.65178	0.71425	-2.58757
C	2.56968	2.13555	-1.21136
H	3.29414	2.56961	-1.91041
H	1.69632	2.79027	-1.17828
H	3.03259	2.17428	-0.21774

E_{SCF}= -1325,222878 au
G_{423}= -1325,104328 au
E_{disp}= -37,8830 kcal·mol^{-1}

17

Ta	0.99381	-0.15622	0.02842
O	-0.21681	1.33305	-0.14770
O	-0.44616	-1.42012	0.13649
Si	-1.82201	1.61116	-0.09583
Si	-2.08267	-1.40145	0.03652
O	-2.58957	0.15652	-0.02762
O	-2.38820	2.33992	-1.45740
H	-2.10904	3.24200	-1.62217
O	-2.12678	2.51296	1.24467
H	-3.04229	2.62811	1.50482
O	-2.79596	-2.05467	1.36423
H	-2.69085	-2.99688	1.50532
O	-2.47299	-2.22397	-1.33380
H	-3.37442	-2.15458	-1.65315
C	2.29155	0.48961	-1.57340
H	2.21110	-1.76878	0.20212
H	2.62670	1.44846	-1.12601
H	1.65868	0.79137	-2.42005
H	1.89142	-1.91162	-0.52588
C	1.95626	-0.09886	1.71904
H	1.39605	-0.61067	2.51703
C	3.21102	0.57360	2.20940
H	3.88347	-0.14189	2.69931
H	3.77402	1.05518	1.40480
H	2.97399	1.34561	2.95234
C	3.50023	-0.30628	-2.07100
H	4.10412	0.26856	-2.78222
H	4.16362	-0.60322	-1.25228
H	3.18804	-1.22164	-2.58376

E_{SCF}= -1325,227242 au
G_{423}= -1325,108301 au
E_{disp}= -37,3649 kcal·mol^{-1}

TS(16-18)

Ta	1.06006	-0.33030	-0.07243
O	-0.03121	1.25405	0.13428
O	-0.53124	-1.39474	-0.17970
Si	-1.59313	1.68248	0.31890
Si	-2.15717	-1.21669	-0.27072
O	-2.52013	0.34373	0.07882
O	-2.10156	2.76792	-0.80760
H	-1.70993	3.64252	-0.78697
O	-1.76573	2.26824	1.84619
H	-2.65540	2.44487	2.15679
O	-2.94003	-2.13038	0.84721
H	-2.96369	-3.07791	0.70475
O	-2.59961	-1.61746	-1.80348
H	-3.47191	-1.35275	-2.10073
C	2.39582	0.74610	-1.40770
H	1.62448	-1.62024	-1.28608
H	1.88906	0.91688	-2.36728
H	3.25436	0.09973	-1.64483
H	1.23080	-0.72453	2.66312
C	1.93268	-0.52272	1.85589
H	2.59958	0.31028	2.08613
C	2.50263	-1.66077	1.12147
H	3.56882	-1.63730	0.90118
H	2.17061	-2.65641	1.41142
H	2.08126	-1.85542	-0.45267
C	2.89244	2.08219	-0.82977
H	3.42475	1.95416	0.11971
H	3.58994	2.58009	-1.51395
H	2.06182	2.76710	-0.64286

E_{SCF}= -1325,239406 au
G_{423}= -1325,117795 au
E_{disp}= -38,6514 kcal·mol^{-1}

18

Ta	1.06388	-0.36166	-0.04969
O	-0.53168	-1.39939	-0.22147
O	0.00243	1.25750	0.09750
Si	-2.15876	-1.19472	-0.27807
Si	-1.55025	1.70287	0.28733
O	-2.49546	0.37282	0.05303
O	-2.93057	-2.08317	0.86719
H	-2.95472	-3.03409	0.74954
O	-2.62726	-1.61826	-1.79689
H	-3.50504	-1.35843	-2.08209
O	-2.05272	2.79056	-0.84050
H	-1.66223	3.66546	-0.81375
O	-1.72484	2.29288	1.81358
H	-2.61538	2.46980	2.12169
H	2.01782	-2.02002	-0.53051
C	2.39991	-1.45641	1.37465
H	2.06278	-2.42532	1.74045

H	3.47288	-1.44534	1.18555
C	1.78237	-0.25864	1.94410
H	2.40827	0.62245	2.09965
H	1.02033	-0.36478	2.71485
H	1.63642	-1.83978	-1.23980
C	2.37874	0.57073	-1.50263
H	3.21012	-0.11393	-1.72724
H	1.83380	0.69518	-2.44935
C	2.93420	1.92589	-1.03475
H	3.61327	2.35877	-1.77877
H	2.13010	2.64407	-0.85770
H	3.50430	1.83984	-0.10298

E_{SCF}= -1325,240956 au
G_{423}= -1325,119368 au
E_{disp}= -38,7401 kcal·mol^{-1}

19

Ta	1.06080	-0.22029	0.04873
O	-0.39582	-1.40295	-0.19257
O	-0.08635	1.34657	0.00578
Si	-2.04117	-1.32676	-0.26112
Si	-1.68210	1.66104	0.10980
O	-2.48999	0.23384	-0.06513
O	-2.75268	-2.16167	0.95899
H	-2.64721	-3.11440	0.97204
O	-2.44923	-1.91680	-1.73793
H	-3.35724	-1.81557	-2.02851
O	-2.22259	2.61649	-1.11403
H	-1.91160	3.52283	-1.13832
O	-1.97909	2.32784	1.58275
H	-2.89402	2.43199	1.85008
C	2.21375	-1.18023	1.56666
H	1.76778	-2.01663	2.10586
H	3.27998	-1.34425	1.39672
C	1.78513	0.19455	1.97816
H	2.55651	0.96938	2.01807
H	1.07289	0.30360	2.79556
C	2.41209	0.04231	-1.58179
H	2.83527	-0.96344	-1.74847
H	1.81855	0.26970	-2.47967
C	3.53525	1.07305	-1.39967
H	4.18577	1.11840	-2.28001
H	3.13613	2.07980	-1.24220
H	4.17356	0.83500	-0.54317

E_{SCF}= -1324,058880 au
G_{423}= -1323,955068 au
E_{disp}= -35,3889 kcal·mol^{-1}

TS(16-20)

Ta	-1.17705	-0.27841	-0.09159
O	-0.15595	1.22271	0.60617
O	0.32106	-1.29444	-0.67078
Si	1.42867	1.62600	0.58752
Si	1.94571	-1.06222	-0.74349
O	2.29584	0.38023	-0.04457
O	2.04410	1.87055	2.09022
H	1.68908	2.59850	2.60293
O	1.54921	2.97072	-0.35471
H	2.42851	3.27400	-0.58803
O	2.48558	-0.94170	-2.29045
H	2.38278	-1.70799	-2.85758
O	2.62737	-2.31930	0.05967
H	3.56610	-2.27761	0.24946
C	-1.61492	-1.41988	1.67794
H	-2.88414	-0.75199	-0.20763
H	-2.12882	-2.35420	1.42643
H	-2.36815	-0.81992	2.21515
H	-2.02091	2.42175	-0.18194
C	-2.63290	1.69443	-0.70059
H	-3.63811	1.52331	-0.33651
C	-2.25567	1.22893	-1.93289
H	-1.33652	1.57650	-2.39859
H	-1.75266	-0.52669	-1.76013
H	-2.96380	0.75153	-2.59821
C	-0.39521	-1.68695	2.57289
H	0.14212	-0.76958	2.83312
H	-0.69642	-2.15913	3.51599
H	0.31857	-2.35722	2.08651

E_{SCF}= -1325,207542 au
G_{423}= -1325,085319 au
E_{disp}= -39,6931 kcal·mol^{-1}

20

Ta	-1.122222	-0.348560	-0.173394
O	-0.140496	1.213443	0.413026
O	0.372688	-1.428535	-0.603720
Si	1.447834	1.617542	0.384471
Si	1.999217	-1.190165	-0.662038
O	2.327387	0.316278	-0.095792
O	2.025965	2.021615	1.865873
H	1.683222	2.816007	2.278451
O	1.572493	2.858562	-0.690065
H	2.449228	3.119646	-0.977580
O	2.571462	-1.213487	-2.200121
H	2.423307	-2.005541	-2.719891
O	2.668866	-2.354030	0.278368
H	3.607784	-2.301258	0.464364
C	-1.587949	-1.416167	1.644978
H	-2.860356	-0.693643	-0.156545
H	-2.118211	-2.345256	1.401733
H	-2.329620	-0.801196	2.177734
H	-2.777793	1.991915	0.447777
C	-3.008228	1.578997	-0.532059
H	-3.988916	1.141015	-0.658198
C	-2.166414	1.749927	-1.572644
H	-1.241969	2.306817	-1.467873
H	-1.759779	-0.741050	-1.768482
H	-2.439932	1.418943	-2.567349
C	-0.373582	-1.694420	2.541264
H	0.170639	-0.779869	2.799638
H	-0.681396	-2.157812	3.486778
H	0.336268	-2.371752	2.059591

E_{SCF}= -1325,213069 au
G_{423}= -1325,092440 au

E_{disp}= -40,0461 kcal·mol^{-1}

3c

Ta	0.974309	-0.427306	-0.050739
O	0.269800	1.215751	0.518322
O	-0.540582	-1.447852	-0.568705
Si	-1.279054	1.817438	0.471098
Si	-2.113667	-0.956695	-0.670894
O	-2.207465	0.587319	-0.108831
O	-1.266791	3.120874	-0.503820
H	-1.862944	3.844039	-0.303562
O	-1.825746	2.283643	1.941184
H	-2.230433	1.631811	2.515994
O	-3.086918	-1.828491	0.320078
H	-3.204590	-2.761173	0.130880
O	-2.537508	-1.064945	-2.246570
H	-3.374386	-0.691568	-2.527750
H	1.501975	-0.330885	-1.715866
H	2.730482	-0.543043	-0.197977
C	1.603202	-1.679256	1.592172
H	2.132174	-2.564361	1.216430
H	2.364714	-1.108662	2.143943
C	0.450354	-2.077556	2.525902
H	-0.098856	-1.206524	2.903788
H	-0.274412	-2.722404	2.021234
H	0.815304	-2.618381	3.407180

E_{SCF}= -1246,627505 au

G_{423}= -1246,554742 au

E_{disp}= -30,0777 kcal·mol^{-1}

V. Reaction of Ta-alkylidenes 6 and 13 with ethene

21_H

Ta	0.855099	-0.113294	-0.245648
O	0.265348	1.682651	0.068118
O	-0.134418	-1.752086	-0.149559
Si	-1.395018	1.755063	0.082485
Si	-1.767180	-1.442833	-0.106533
O	-1.846077	0.172499	0.230633
O	-1.979774	2.487482	-1.261848
H	-1.561008	2.249068	-2.092560
O	-1.983179	2.553209	1.378156
H	-2.252958	3.464182	1.252479
O	-2.529493	-2.228861	1.102961
H	-2.992792	-3.038523	0.883370
O	-2.496313	-1.862151	-1.512942
H	-2.028071	-1.635415	-2.320094
C	2.725697	-0.364983	-0.755859
C	3.943604	0.473071	-0.992605
H	2.901327	-1.442936	-0.919114
H	4.287799	0.362281	-2.028479
H	3.762450	1.536798	-0.816641
H	0.058354	0.082312	-1.850988
H	4.780250	0.160068	-0.353784
C	2.277513	-0.430329	1.914213
H	2.734047	-1.411460	1.846301
H	2.963982	0.409637	1.917378
C	0.959819	-0.276319	2.247404
H	0.574501	0.694387	2.539369
H	0.339355	-1.139895	2.460377

E_{SCF}= -1324,008026 au

G_{423}= -1323,904897 au

E_{disp}= -39,0056 kcal·mol^{-1}

TS(21_H-22_H)

Ta	0.804508	-0.118346	-0.197275
O	0.236751	1.691670	0.054768
O	-0.171128	-1.763963	-0.118744
Si	-1.426598	1.750638	0.074747
Si	-1.802327	-1.434387	-0.087625
O	-1.854872	0.170259	0.315237
O	-2.025231	2.404564	-1.304354
H	-1.618119	2.094983	-2.117844
O	-2.014282	2.615046	1.326603
H	-2.315965	3.506200	1.144294
O	-2.591293	-2.258936	1.077516
H	-3.089041	-3.033075	0.810327
O	-2.519100	-1.789044	-1.518832
H	-2.042109	-1.500576	-2.301505
C	2.716774	-0.385266	-0.633652
C	3.909513	0.491454	-0.870439
H	2.932779	-1.453932	-0.786993
H	4.214947	0.408292	-1.920281
H	3.703489	1.546149	-0.670069
H	-0.121255	0.071387	-1.767425
H	4.774443	0.186698	-0.268080
C	2.434435	-0.440987	1.661442
H	2.893955	-1.423384	1.668661
H	3.132075	0.387017	1.731054
C	1.109274	-0.278917	2.101580
H	0.811077	0.677556	2.518452
H	0.556204	-1.147250	2.443407

E_{SCF}= -1324,007560 au

G_{423}= -1323,900822 au

E_{disp}= -39,4209 kcal·mol^{-1}

22_H

Ta	0.785402	-0.154149	-0.238840
O	0.267486	1.671747	-0.024117
O	-0.202329	-1.786763	-0.172659
Si	-1.395412	1.745690	0.106343
Si	-1.826649	-1.424503	-0.029016
O	-1.847631	0.177911	0.386321
O	-2.067899	2.406426	-1.235683
H	-1.731801	2.075098	-2.072358
O	-1.884521	2.629195	1.386496
H	-2.159136	3.532178	1.220409
O	-2.547392	-2.248773	1.178995
H	-3.039899	-3.036342	0.943232
O	-2.635664	-1.768924	-1.413548

H	-2.213884	-1.472161	-2.223915
C	2.829071	-0.443473	-0.303888
C	3.932889	0.426611	-0.876841
H	3.023276	-1.509668	-0.483671
H	4.051969	0.236585	-1.946807
H	3.714063	1.491466	-0.752600
H	-0.311853	0.062838	-1.709622
H	4.898610	0.228679	-0.395660
C	2.644375	-0.246187	1.314870
H	3.217777	-1.054156	1.768302
H	3.106281	0.714000	1.545982
C	1.184967	-0.268186	1.857150
H	0.954592	0.586688	2.487469
H	0.921222	-1.209049	2.337934

E_{SCF}= -1324,016625 au
G_{423}= -1323,907015 au
E_{disp}= -39,1482 kcal·mol^{-1}

TS(22_H-23_H)

Ta	-0.820528	-0.142573	0.000537
O	-0.091670	1.552621	-0.313568
O	0.274387	-1.672793	-0.050383
Si	1.575275	1.691960	-0.111789
Si	1.920282	-1.406588	0.140914
O	2.153237	0.164407	-0.297024
O	1.894436	2.378045	1.339571
H	1.424941	1.965714	2.072895
O	2.239079	2.614204	-1.277289
H	2.337623	3.551279	-1.102277
O	2.803353	-2.324752	-0.873153
H	3.079773	-3.188937	-0.564606
O	2.362549	-1.756672	1.678265
H	1.788937	-1.359927	2.342884
C	-2.759330	-0.318519	0.698542
C	-3.538151	0.666096	1.549812
H	-2.916357	-1.354285	1.028857
H	-3.270200	0.553589	2.603225
H	-3.328656	1.702126	1.265718
H	0.143272	0.093321	1.665215
H	-4.620606	0.512697	1.459859
C	-3.084115	-0.230565	-0.876408
H	-3.831066	-0.999103	-1.076608
H	-3.520093	0.755032	-1.048795
C	-1.856819	-0.436754	-1.852194
H	-1.843225	0.316387	-2.637961
H	-1.852299	-1.437817	-2.285569

E_{SCF}= -1324,012360 au
G_{423}= -1323,904066 au
E_{disp}= -37,9761 kcal·mol^{-1}

23_H

Ta	-1.005619	-0.210865	-0.021874
O	0.488484	-1.438855	0.140742
O	0.064721	1.327650	-0.157887
Si	2.118103	-1.348340	0.001960
Si	1.682254	1.682345	-0.131405
O	2.471101	0.247088	-0.232825
O	2.647251	-2.272754	-1.251697
H	2.014762	-2.466899	-1.945673
O	2.931797	-1.812004	1.342661
H	3.136381	-2.743802	1.433988
O	1.930898	2.482073	1.270033
H	2.777282	2.910798	1.406618
O	2.149449	2.646283	-1.370077
H	2.402423	2.230942	-2.196114
C	-2.980826	0.491403	-0.505835
C	-4.126057	-0.348601	-1.041852
H	-2.923355	1.456945	-1.021744
H	-3.995432	-0.535399	-2.111246
H	-4.180224	-1.327802	-0.552978
H	-1.282106	-1.138356	-1.479642
H	-5.101232	0.137794	-0.902671
C	-3.014252	0.690355	1.051414
H	-2.637723	1.672722	1.354171
H	-4.052225	0.632595	1.393557
C	-2.162958	-0.449699	1.709646
H	-2.732684	-1.382664	1.771343
H	-1.740204	-0.200263	2.683882

E_{SCF}= -1324,043237 au
G_{423}= -1323,937086 au
E_{disp}= -36,2630 kcal·mol^{-1}

TS(23_H-24_H)

Ta	1.038756	-0.256094	-0.236565
O	-0.505427	-1.376684	-0.029858
O	-0.060455	1.316484	0.029007
Si	-2.141502	-1.258928	0.093302
Si	-1.639089	1.742358	0.195499
O	-2.471213	0.328243	0.366900
O	-2.679040	-2.224244	1.309881
H	-2.065357	-2.435330	2.014802
O	-2.941494	-1.676495	-1.270350
H	-3.085247	-2.609788	-1.434442
O	-2.045397	2.583872	-1.145121
H	-2.886950	3.042556	-1.153381
O	-1.945415	2.679170	1.509368
H	-2.180865	2.236102	2.325867
C	2.659710	0.319573	0.927581
C	3.572605	-0.534177	1.785523
H	2.422186	1.272514	1.414047
H	3.111715	-0.724873	2.758897
H	3.769076	-1.498155	1.311343
H	1.992211	-1.794402	-0.541464
H	4.532674	-0.036904	1.970930
C	3.239433	0.633669	-0.544182
H	3.605042	1.659346	-0.516586
H	4.054297	-0.067512	-0.707956
C	2.229786	0.517630	-1.758572
H	2.599817	-0.144653	-2.536878
H	1.940509	1.491350	-2.154505

E_{SCF}= -1324,036985 au

G_{423}= -1323,928435 au
E_{disp}= -36,1087 kcal·mol^{-1}

24_H

Ta	-1.075039	0.003134	-0.233407
O	0.315274	1.359873	-0.038438
O	0.166773	-1.375420	0.094531
Si	1.951592	1.427768	-0.009703
Si	1.798141	-1.610036	0.177251
O	2.469630	-0.113281	0.269592
O	2.449657	2.462413	1.169332
H	1.893649	2.546591	1.945082
O	2.658655	1.894444	-1.408681
H	2.615886	2.822126	-1.645015
O	2.214475	-2.450377	-1.158205
H	3.093262	-2.830592	-1.200472
O	2.253726	-2.476174	1.494629
H	2.453265	-1.993690	2.298229
C	-2.603930	0.371414	1.122125
C	-3.022913	1.653989	0.430115
H	-2.596995	0.384972	2.207014
H	-2.739193	2.534795	1.007436
H	-2.527812	1.778069	-0.574206
H	-1.237537	0.756207	-1.803508
H	-4.090291	1.693257	0.184560
C	-3.281881	-0.893502	0.483995
H	-3.134719	-1.743605	1.153362
H	-4.356812	-0.699893	0.402048
C	-2.707997	-1.190966	-0.952851
H	-3.372609	-0.842871	-1.741687
H	-2.493648	-2.251272	-1.094828

E_{SCF}= -1324,045034 au

G_{423}= -1323,937674 au

E_{disp}= -37,0014 kcal·mol^{-1}

TS(24_H-25_H)

Ta	-0.902180	-0.409112	-0.433677
O	-0.285815	1.466314	-0.317341
O	0.234666	-1.747169	0.185754
Si	1.336858	1.680361	-0.198327
Si	1.850259	-1.378379	0.455473
O	1.965372	0.256250	0.386667
O	1.636858	2.915506	0.850740
H	0.948789	3.098202	1.492734
O	2.158098	2.013828	-1.573121
H	2.170336	2.928122	-1.860077
O	2.690183	-2.201395	-0.669311
H	3.638145	-2.286860	-0.556672
O	2.341134	-1.874146	1.939312
H	2.256038	-1.253821	2.665139
C	-2.078643	0.125791	1.275535
C	-2.176041	1.396999	2.077905
H	-2.031132	-0.769364	1.916026
H	-1.401518	1.420950	2.851073
H	-2.021518	2.264133	1.426785
H	0.195856	-0.187788	-1.851324
H	-3.142065	1.518569	2.585472
C	-3.237250	-0.077936	0.221296
H	-4.033649	-0.669786	0.676074
H	-3.623307	0.910015	-0.036186
C	-2.815197	-0.814018	-1.132798
H	-3.211590	-0.299658	-2.007933
H	-3.116465	-1.864540	-1.143750

E_{SCF}= -1324,006222 au

G_{423}= -1323,899123 au

E_{disp}= -38,2559 kcal·mol^{-1}

25_H

Ta	-0.850158	-0.287873	-0.539916
O	-0.436057	1.584624	-0.541901
O	0.165289	-1.811311	0.017316
Si	1.178833	1.778753	-0.205482
Si	1.720445	-1.319262	0.377480
O	1.643900	0.332054	0.486941
O	1.468772	2.961123	0.897370
H	1.280343	2.772742	1.817852
O	1.988667	2.196241	-1.556727
H	2.804981	2.685823	-1.442509
O	2.859284	-1.740038	-0.711466
H	3.307798	-2.575585	-0.571109
O	2.170430	-1.981833	1.813245
H	1.492583	-2.120307	2.476155
C	-1.653192	-0.024941	1.434521
C	-1.500323	1.154207	2.366531
H	-1.555387	-0.978604	1.965561
H	-0.558715	1.086427	2.921622
H	-1.500180	2.093807	1.805335
H	0.501616	-0.229311	-1.716943
H	-2.305446	1.207478	3.110948
C	-2.993119	-0.030889	0.607765
H	-3.718551	-0.656986	1.129029
H	-3.369900	0.992179	0.557334
C	-2.878075	-0.596999	-0.890824
H	-3.434506	0.026397	-1.590564
H	-3.222864	-1.631784	-0.954554

E_{SCF}= -1324,011331 au

G_{423}= -1323,901530 au

E_{disp}= -40,3769 kcal·mol^{-1}

TS(25_H-26)

Ta	-0.861889	-0.189889	-0.543870
O	-0.234053	1.613909	-0.454285
O	0.007339	-1.783651	0.069321
Si	1.407335	1.651348	-0.163777
Si	1.622363	-1.504828	0.363300
O	1.730206	0.144362	0.435509
O	1.742373	2.825889	0.935066
H	1.078038	3.027311	1.595480
O	2.346519	1.945060	-1.461596
H	2.640456	2.848417	-1.589518
O	2.645005	-2.083269	-0.764235
H	3.055855	-2.931192	-0.588499
O	2.059885	-2.194697	1.788748
H	1.444150	-2.174629	2.522063
C	-1.707841	0.054067	1.697408
C	-1.501481	1.411175	2.328279

H	-1.224466	-0.783112	2.195525
H	-0.457139	1.555562	2.619675
H	-1.778638	2.222106	1.649541
H	0.338067	-0.305626	-1.858944
H	-2.103523	1.513960	3.239226
C	-2.887759	-0.252469	1.003772
H	-3.267469	-1.267510	1.002520
H	-3.639224	0.514572	0.845246
C	-2.668038	-0.422838	-1.302532
H	-3.279341	0.413256	-1.653327
H	-3.167738	-1.382289	-1.452927

E_{SCF}= -1323,993690 au
G_{423}= -1323,888502 au
E_{disp}= -40,1636 kcal·mol^{-1}

26

Ta	-1.351910	0.002721	-0.222784
O	-0.256395	-1.528992	-0.116779
O	-0.249071	1.527583	-0.073113
Si	1.393868	-1.563023	0.049216
Si	1.405309	1.549833	0.036320
O	1.925585	-0.008601	0.059795
O	2.119948	-2.271696	-1.234330
H	1.941919	-3.198358	-1.404464
O	1.687590	-2.326963	1.464931
H	2.577721	-2.317107	1.820758
O	1.917741	2.209327	1.443643
H	1.667473	3.113532	1.641539
O	1.931101	2.353038	-1.287498
H	2.874090	2.411970	-1.449766
C	-2.878212	-0.008014	0.939282
H	-3.320937	0.902899	1.353408
H	-2.216531	0.021525	-1.756055
H	-3.320006	-0.917933	1.355453

E_{SCF}= -1206,108891 au
G_{423}= -1206,078767 au
E_{disp}= -23,5234 kcal·mol^{-1}

21_{Me}

Ta	0.963001	-0.120835	-0.468535
O	0.299407	1.658522	-0.171263
O	-0.058349	-1.741412	-0.306879
Si	-1.345139	1.731775	0.010833
Si	-1.683664	-1.483812	-0.118330
O	-1.830820	0.156790	-0.047964
O	-2.041711	2.657882	-1.147626
H	-1.687169	2.609829	-2.037521
O	-1.798926	2.339353	1.458319
H	-2.065095	3.259620	1.488549
O	-2.268374	-2.097951	1.278388
H	-2.712821	-2.946136	1.236748
O	-2.544024	-2.150160	-1.343532
H	-2.174300	-2.108353	-2.227506
C	2.877942	-0.396304	-0.637487
C	4.153840	0.385610	-0.701531
H	3.023134	-1.489748	-0.722094
H	4.677876	0.206151	-1.648986
H	3.984552	1.463226	-0.619940
H	4.849466	0.096486	0.098154
C	2.006694	-0.318758	2.033358
H	2.494460	-1.286901	2.037014
H	2.664192	0.543947	2.057183
C	0.666878	-0.194947	2.195997
H	0.211209	0.774026	2.367415
H	0.037503	-1.067190	2.334638
C	0.412396	0.042821	-2.585025
H	0.933265	0.890028	-3.048185
H	0.709827	-0.850149	-3.147341
H	-0.665591	0.192661	-2.753856

E_{SCF}= -1363,325428 au
G_{423}= -1363,199934 au
E_{disp}= -45,1737 kcal·mol^{-1}

TS(21_{Me}-22_{Me})

Ta	0.821948	-0.128922	-0.225841
O	0.228348	1.689438	-0.036983
O	-0.190453	-1.761425	-0.146710
Si	-1.416953	1.772294	0.140921
Si	-1.807097	-1.456187	0.055239
O	-1.886769	0.189770	0.145235
O	-2.110946	2.642956	-1.062555
H	-1.757964	2.536868	-1.948304
O	-1.884508	2.444335	1.553527
H	-2.179701	3.355883	1.530034
O	-2.415492	-2.066042	1.442543
H	-2.906340	-2.887159	1.383794
O	-2.692937	-2.076029	-1.177226
H	-2.319579	-2.029765	-2.059657
C	2.776620	-0.434211	-0.237675
C	4.017168	0.407460	-0.283151
H	2.985391	-1.513540	-0.301014
H	4.518927	0.266402	-1.247836
H	3.803550	1.474537	-0.176451
H	4.740685	0.123888	0.491775
C	2.099865	-0.362481	1.931064
H	2.556264	-1.335568	2.077368
H	2.770564	0.476918	2.083539
C	0.719300	-0.195248	2.137466
H	0.359602	0.771689	2.472787
H	0.128752	-1.053730	2.438932
C	0.215506	0.019363	-2.358105
H	0.744459	0.856783	-2.834174
H	0.516930	-0.887835	-2.899306
H	-0.855996	0.166455	-2.561623

E_{SCF}= -1363,324386 au
G_{423}= -1363,193294 au
E_{disp}= -45,5889 kcal·mol^{-1}

22_{Me}

Ta	0.887015	-0.174951	-0.503137
O	0.337416	1.656917	-0.329654
O	-0.134138	-1.794902	-0.410932
Si	-1.282715	1.748019	0.025251
Si	-1.723447	-1.463371	-0.052245

O	-1.810295	0.184601	-0.021155
O	-2.061123	2.704667	-1.056755
H	-1.784353	2.656813	-1.973645
O	-1.595921	2.354054	1.509144
H	-1.837705	3.280253	1.558964
O	-2.198569	-2.031715	1.402419
H	-2.678432	-2.861371	1.411663
O	-2.720770	-2.123364	-1.175245
H	-2.438520	-2.101407	-2.091425
C	2.906908	-0.461480	-0.162026
C	4.108924	0.346677	-0.616359
H	3.108206	-1.540962	-0.218836
H	4.406635	0.059812	-1.628493
H	3.893907	1.419617	-0.625827
H	4.974084	0.190581	0.040184
C	2.458453	-0.125825	1.369294
H	2.990941	-0.847769	1.990060
H	2.830698	0.878608	1.576991
C	0.934106	-0.194611	1.668613
H	0.586318	0.657370	2.247678
H	0.642002	-1.133411	2.138770
C	0.113001	-0.011216	-2.578359
H	0.616193	0.835361	-3.069532
H	0.411725	-0.924586	-3.116192
H	-0.963435	0.116987	-2.750526

E_{SCF}= -1363,334277 au
G_{423}= -1363,201866 au
E_{disp}= -45,2258 kcal·mol^{-1}

TS(22_{Me}-23_{Me})

Ta	-0.827538	-0.086253	0.441837
O	-0.141959	1.627143	0.143304
O	0.342645	-1.656138	0.468200
Si	1.485357	1.755511	-0.262250
Si	1.867929	-1.418963	-0.084110
O	2.049120	0.226723	-0.199351
O	2.230760	2.773851	0.780792
H	2.100652	2.655644	1.723275
O	1.681418	2.365632	-1.759842
H	1.859246	3.304305	-1.837380
O	2.186287	-2.032268	-1.566761
H	2.632606	-2.879865	-1.595145
O	2.964404	-2.074130	0.951608
H	2.697231	-2.150397	1.869359
C	-2.887063	-0.303902	0.320667
C	-3.947162	0.656165	0.829674
H	-3.159865	-1.349596	0.518434
H	-4.132490	0.500312	1.895567
H	-3.648470	1.700927	0.695091
H	-4.899820	0.520574	0.302066
C	-2.583312	-0.162191	-1.253788
H	-3.293009	-0.825150	-1.753092
H	-2.810908	0.867916	-1.540400
C	-1.128266	-0.544665	-1.669715
H	-0.735683	0.123161	-2.435904
H	-1.048701	-1.580688	-1.999251
C	-0.292056	-0.080627	2.602692
H	-0.778789	0.756317	3.127511
H	-0.653071	-1.012100	3.061620
H	0.781435	-0.027607	2.830873

E_{SCF}= -1363,330509 au
G_{423}= -1363,200412 au
E_{disp}= -43,6180 kcal·mol^{-1}

23_{Me}

Ta	-0.936024	-0.177324	-0.399679
O	0.488689	-1.468255	-0.146786
O	0.146261	1.367686	-0.416147
Si	2.100293	-1.343616	0.141933
Si	1.743811	1.695206	-0.140693
O	2.504869	0.240499	-0.076472
O	2.937569	-2.325330	-0.876620
H	2.516484	-2.569321	-1.702123
O	2.534788	-1.715876	1.674542
H	2.636054	-2.642846	1.895833
O	1.789427	2.533458	1.259097
H	2.608697	2.965338	1.506189
O	2.430550	2.608057	-1.314874
H	2.818819	2.160875	-2.068451
C	-3.002430	0.483069	-0.471295
C	-4.226460	-0.347245	-0.810452
H	-3.041647	1.454738	-0.986318
H	-4.285609	-0.539371	-1.886154
H	-4.208257	-1.322572	-0.310995
H	-5.160725	0.148782	-0.513140
C	-2.773280	0.649846	1.062854
H	-2.259977	1.588144	1.308035
H	-3.726402	0.684780	1.606160
C	-1.907082	-0.574258	1.446691
H	-2.506028	-1.487091	1.503290
H	-1.298848	-0.471950	2.349027
C	-1.325703	-1.146940	-2.289397
H	-1.911195	-2.053224	-2.075719
H	-1.912173	-0.535678	-2.981677
H	-0.401067	-1.462727	-2.786482

E_{SCF}= -1363,364527 au
G_{423}= -1363,233324 au
E_{disp}= -41,6790 kcal·mol^{-1}

TS(23_{Me}-24_{Me})

Ta	0.953079	-0.230710	-0.203191
O	-0.571704	-1.402906	-0.049046
O	-0.262907	1.270672	0.053945
Si	-2.210010	-1.381984	0.051639
Si	-1.855653	1.629268	0.170710
O	-2.639098	0.182888	0.313247
O	-2.717124	-2.376350	1.260787
H	-2.129948	-2.508220	2.006202
O	-2.964487	-1.865993	-1.317699
H	-3.116696	-2.805636	-1.428601
O	-2.258464	2.458475	-1.181278
H	-3.113971	2.890038	-1.203687
O	-2.254474	2.551692	1.472461
H	-2.508246	2.094824	2.275684

C	2.389214	0.670187	1.022613
C	3.452053	0.049820	1.907672
H	1.927741	1.533418	1.509377
H	3.016344	-0.265490	2.860168
H	3.907748	-0.827468	1.443511
H	4.250126	0.766570	2.138118
C	2.920733	1.136835	-0.424934
H	2.988373	2.222858	-0.398944
H	3.906683	0.690947	-0.543318
C	2.047575	0.740777	-1.688930
H	2.610094	0.144371	-2.403899
H	1.584144	1.605336	-2.160441
C	2.216100	-2.019237	-0.400428
H	2.124939	-2.673493	0.479143
H	1.832331	-2.607535	-1.249399
H	3.286501	-1.862335	-0.579742

E_{SCF}= -1363,362269 au
G_{423}= -1363,228195 au
E_{disp}= -41,3950 kcal·mol^{-1}

24_{Me}

Ta	-0.927749	0.170213	-0.333429
O	0.595016	1.381888	-0.330318
O	0.251732	-1.161652	0.396172
Si	2.232262	1.374562	-0.260272
Si	1.845787	-1.528667	0.493665
O	2.661367	-0.106944	0.313538
O	2.760308	2.596041	0.709441
H	2.208605	2.842434	1.452942
O	2.981342	1.555694	-1.705014
H	3.096025	2.448158	-2.034728
O	2.170193	-2.613449	-0.687040
H	3.039532	-3.016825	-0.703475
O	2.275109	-2.197446	1.931456
H	2.507618	-1.602211	2.645515
C	-2.555467	0.351401	0.934917
C	-3.447984	1.570793	1.101336
H	-2.340283	-0.122933	1.898980
H	-2.998239	2.287470	1.793744
H	-3.614613	2.086747	0.151188
H	-4.431128	1.295389	1.502682
C	-3.158021	-0.767749	-0.061979
H	-3.562578	-1.555713	0.572815
H	-3.966446	-0.285741	-0.612159
C	-2.147920	-1.402065	-1.087301
H	-2.544167	-1.407091	-2.098507
H	-1.829367	-2.398551	-0.783554
C	-1.491931	1.204142	-2.157277
H	-1.394345	2.283307	-1.966156
H	-0.831193	0.971097	-3.000256
H	-2.518854	0.995773	-2.480712

E_{SCF}= -1363,365874 au
G_{423}= -1363,234306 au
E_{disp}= -41,1954 kcal·mol^{-1}

TS(24_{Me}-25_{Me})

Ta	-0.839584	-0.485118	-0.518487
O	-0.249570	1.398279	-0.634850
O	0.249074	-1.789770	0.263001
Si	1.287416	1.701602	-0.160009
Si	1.783928	-1.334108	0.742652
O	1.851440	0.287826	0.504317
O	1.330226	2.933984	0.930606
H	0.535075	3.060988	1.451728
O	2.349456	2.082965	-1.346677
H	2.401002	3.003612	-1.607863
O	2.822196	-2.200438	-0.164447
H	3.737359	-2.252983	0.115475
O	2.072241	-1.665896	2.321120
H	1.820288	-1.009179	2.972312
C	-1.812330	0.207092	1.303620
C	-1.794147	1.514655	2.054123
H	-1.737688	-0.653031	1.986626
H	-0.928188	1.568020	2.723574
H	-1.737634	2.352693	1.348972
H	-2.684335	1.672377	2.678629
C	-3.086730	0.011341	0.406782
H	-3.883644	-0.446867	0.998713
H	-3.422492	0.996122	0.072290
C	-2.849130	-0.902190	-0.871613
H	-3.357813	-0.513242	-1.753625
H	-3.147577	-1.939770	-0.695654
C	0.227279	-0.542928	-2.431522
H	0.190802	-1.583603	-2.791651
H	-0.348888	0.082344	-3.129886
H	1.264433	-0.199587	-2.492673

E_{SCF}= -1363,330040 au
G_{423}= -1363,196789 au
E_{disp}= -44,9598 kcal·mol^{-1}

25_{Me}

Ta	-0.985558	-0.277506	-0.679473
O	-0.463201	1.571325	-0.597413
O	0.034280	-1.830781	-0.222240
Si	1.145062	1.745086	-0.252463
Si	1.572561	-1.422386	0.265872
O	1.634432	0.222353	0.196888
O	1.466285	2.801821	0.960165
H	1.188743	2.575077	1.849014
O	1.937786	2.302765	-1.564988
H	2.728493	2.822750	-1.411881
O	2.758966	-1.998617	-0.694203
H	3.070820	-2.890112	-0.531331
O	1.844646	-1.993727	1.782126
H	1.100335	-2.022043	2.385491
C	-1.511994	-0.061010	1.435694
C	-1.200727	1.038109	2.425533
H	-1.428002	-1.050201	1.903809
H	-0.204738	0.898274	2.862115
H	-1.230943	2.018351	1.937554
H	-1.908181	1.070241	3.265467
C	-2.938917	0.062147	0.794218
H	-3.653513	-0.493473	1.405581
H	-3.226935	1.115841	0.787124

C	-3.054644	-0.501822	-0.696711
H	-3.688660	0.131560	-1.317476
H	-3.429419	-1.528847	-0.709011
C	0.099374	-0.309314	-2.579288
H	-0.148445	-1.294433	-3.008966
H	-0.367113	0.464162	-3.208781
H	1.181343	-0.182884	-2.671849

E_{SCF}= -1363,331337 au
G_{423}= -1363,199011 au
E_{disp}= -46,6092 kcal·mol^{-1}

TS(25_{Me}-10)

Ta	-0.906849	-0.170165	-0.486487
O	-0.155704	1.590645	-0.482738
O	-0.055017	-1.751155	0.199566
Si	1.478675	1.609637	-0.173386
Si	1.548899	-1.526758	0.564782
O	1.785979	0.098497	0.409297
O	1.843216	2.796859	0.899210
H	1.180446	3.034423	1.549336
O	2.418888	1.858145	-1.482343
H	2.713765	2.755299	-1.645973
O	2.590228	-2.286957	-0.432745
H	2.857867	-3.177723	-0.201913
O	1.869976	-2.058383	2.085141
H	1.204913	-1.946320	2.765197
C	-1.470695	0.228859	1.885304
C	-1.137435	1.595697	2.432780
H	-0.978411	-0.611304	2.367775
H	-0.068461	1.677264	2.651554
H	-1.407184	2.391801	1.732793
H	-1.666456	1.786555	3.374788
C	-2.730944	-0.044647	1.342070
H	-3.153188	-1.038753	1.429625
H	-3.462106	0.751137	1.241449
C	-2.820843	-0.300908	-0.944652
H	-3.416068	0.565107	-1.246798
H	-3.399817	-1.225752	-0.982849
C	0.135636	-0.545828	-2.369194
H	-0.179773	-1.530406	-2.739990
H	-0.191242	0.198200	-3.107659
H	1.231127	-0.539089	-2.365969

E_{SCF}= -1363,312952 au
G_{423}= -1363,182132 au
E_{disp}= -46,4285 kcal·mol^{-1}

VI. Hydrogenation of propene and Ta-methylidene

27

Ta	-0.772488	-0.899696	-0.104522
O	-0.514745	1.003533	-0.238192
O	0.992496	-1.446105	0.158330
Si	0.816783	1.963696	-0.163343
Si	2.439083	-0.632798	0.225494
O	2.119291	0.960136	0.038149
O	0.626643	2.979694	1.100715
H	1.114647	3.804490	1.089737
O	1.051428	2.875448	-1.505209
H	1.463424	2.471085	-2.270626
O	3.413876	-1.045468	-1.024281
H	3.704276	-1.956732	-1.094289
O	3.076180	-0.987433	1.689196
H	3.872422	-0.534378	1.971149
C	-3.242882	0.069022	-0.995293
H	-2.880437	0.957682	-1.503761
H	-3.461237	-0.802256	-1.599952
C	-3.526719	0.088655	0.320281
H	-3.938715	-0.812247	0.767999
H	-1.599636	-1.239408	1.404591
H	-1.098575	-1.386264	-1.754896
H	-1.929811	-2.236192	-0.225187
C	-3.429107	1.287640	1.206412
H	-4.441071	1.629824	1.455817
H	-2.934258	1.047875	2.151220
H	-2.893292	2.107474	0.726664

E_{SCF}= -1285,904288 au
G_{423}= -1285,810721 au
E_{disp}= -34,6521 kcal·mol^{-1}

TS(27-28)

Ta	-0.998016	-0.335385	-0.631961
O	0.009131	1.298781	-0.400328
O	0.392058	-1.484769	-0.062788
Si	1.515016	1.717097	0.079615
Si	1.947978	-1.291511	0.438729
O	2.311249	0.305951	0.409871
O	1.376624	2.660433	1.411182
H	2.100320	3.257738	1.606462
O	2.364956	2.576948	-1.029055
H	2.734985	2.111607	-1.781188
O	3.014372	-2.009118	-0.581586
H	2.920872	-2.950652	-0.736738
O	2.015724	-1.909433	1.958004
H	2.844748	-1.841287	2.434587
C	-2.728317	1.216359	0.174048
H	-2.162870	1.976244	0.701608
H	-3.104820	1.467684	-0.814642
C	-3.231196	0.133536	0.844177
H	-3.968734	-0.488497	0.348264
H	-2.062506	-1.319771	0.410202
H	-0.628116	-0.579863	-2.316105
H	-2.429710	-0.790802	-1.580225
C	-3.087395	-0.049730	2.322923
H	-3.972690	0.385324	2.803195
H	-3.038952	-1.102717	2.603320
H	-2.209453	0.467421	2.716290

E_{SCF}= -1285,897327 au
G_{423}= -1285,799973 au
E_{disp}= -34,0036 kcal·mol^{-1}

28

Ta	0.766801	-0.484707	-0.648962

O	-0.606374	-1.586577	0.005207
O	0.135743	1.291503	-0.439321
Si	-2.114033	-1.165608	0.564841
Si	-1.318048	1.799097	0.158070
O	-2.195747	0.470502	0.576563
O	-2.329396	-1.639409	2.116006
H	-2.369276	-2.578516	2.305183
O	-3.179818	-1.844986	-0.472457
H	-4.100145	-1.579435	-0.433122
O	-2.216859	2.575827	-0.968112
H	-1.832472	3.332484	-1.414354
O	-0.968665	2.722937	1.463108
H	-1.691255	3.059195	1.995855
C	2.396653	-0.382356	0.750025
H	1.947774	0.080096	1.649037
H	2.615848	-1.427622	1.023721
C	3.691275	0.342025	0.380807
H	4.142939	-0.156942	-0.483167
H	3.461086	1.364674	0.055222
H	0.652655	-0.350390	-2.392616
H	2.123135	-1.262080	-1.466121
C	4.704153	0.405034	1.524748
H	5.616286	0.929363	1.221810
H	4.289782	0.929435	2.391864
H	4.989244	-0.600421	1.851264

E_{SCF}= -1285,938883 au
G_{423}= -1285,841877 au
E_{disp}= -32,4849 kcal·mol^{-1}

29

Ta	0.825935	-0.189703	-0.731700
O	-0.437177	-1.452875	-0.145584
O	-0.170213	1.403294	-0.305307
Si	-1.984690	-1.380819	0.442819
Si	-1.670507	1.659199	0.304134
O	-2.365628	0.199679	0.623924
O	-2.087703	-2.052282	1.933375
H	-2.000857	-3.004293	2.006243
O	-2.925909	-2.140508	-0.660440
H	-3.875123	-2.012220	-0.621698
O	-2.682454	2.383250	-0.765642
H	-2.408215	3.218865	-1.147279
O	-1.465637	2.533597	1.676497
H	-2.239215	2.729301	2.207844
C	2.440159	-0.142974	0.685002
H	1.979187	0.288511	1.591240
H	2.425501	-1.241204	0.854562
C	3.884921	0.323636	0.543056
H	4.304846	-0.090496	-0.380103
H	3.899608	1.414582	0.425379
H	0.567017	0.195568	-2.424214
H	2.029396	-1.029826	-1.761147
C	4.772589	-0.060071	1.726165
H	5.797610	0.298602	1.589020
H	4.391856	0.364634	2.660705
H	4.813902	-1.147251	1.849552
H	1.873892	1.216089	-1.888618
H	2.331486	1.229480	-1.256370

E_{SCF}= -1287,119821 au
G_{423}= -1287,007247 au
E_{disp}= -34,7646 kcal·mol^{-1}

TS(29-1b)

Ta	-0.764722	-0.602532	-0.494819
O	-0.081215	1.189861	-0.379110
O	0.834651	-1.473022	0.035890
Si	1.381727	1.852103	-0.037210
Si	2.340952	-0.990901	0.497446
O	2.422613	0.640443	0.353052
O	1.323127	2.820250	1.288571
H	0.854870	3.653092	1.210062
O	1.864612	2.663184	-1.377748
H	2.786198	2.917897	-1.445914
O	3.509076	-1.591855	-0.480934
H	3.620591	-2.543190	-0.520306
O	2.508872	-1.474106	2.056671
H	3.271256	-1.162635	2.547602
C	-2.677120	0.307462	0.455023
C	-4.086671	-0.229661	0.701369
H	-4.372486	-0.870476	-0.139230
H	-4.085035	-0.876427	1.588862
H	-0.571870	-0.723126	-2.217047
H	-2.104121	-1.449523	-1.298211
H	-1.541659	-1.848054	0.704100
H	-2.684262	0.928724	-0.459322
H	-2.350755	0.958220	1.275088
H	-2.095158	-1.066150	0.709362
C	-5.123319	0.875574	0.891707
H	-6.118804	0.457469	1.069357
H	-4.871386	1.513398	1.744876
H	-5.183664	1.515455	0.005675

E_{SCF}= -1287,095883 au
G_{423}= -1286,980999 au
E_{disp}= -34,7169 kcal·mol^{-1}

TS(28-1a)

Ta	-0.759626	-0.243371	-0.732859
O	0.439760	-1.546873	-0.104659
O	0.104398	1.402840	-0.455796
Si	1.934251	-1.339740	0.575559
Si	1.609816	1.697456	0.164154
O	2.271400	0.266575	0.625341
O	3.122003	-2.013602	-0.330374
H	3.057498	-2.947246	-0.538143
O	1.837593	-1.991429	2.076202
H	2.589845	-1.892509	2.662234
O	1.536345	2.610448	1.524146
H	1.241338	3.518389	1.436620
O	2.468307	2.421237	-1.028455
H	3.421878	2.463623	-0.940880
C	-3.079493	-0.603353	0.015831
H	-3.985882	-0.924378	-0.530626
H	-2.774733	-1.479203	0.598244
H	-1.400136	-0.493524	-2.358694

H	-2.538588	-0.499509	-1.111530
C	-3.472992	0.573314	0.913076
H	-2.687534	0.733733	1.657596
H	-3.520443	1.493010	0.317789
C	-4.822433	0.359931	1.601920
H	-5.072373	1.207869	2.246303
H	-5.630324	0.247416	0.871810
H	-4.808968	-0.539168	2.226195

E_{SCF}= -1285,875406 au
G_{423}= -1285,777219 au
E_{disp}= -31,6841 kcal·mol^{-1}

TS(26-30a)

Ta	-0.970817	-0.189045	-0.443615
O	0.144359	1.370163	-0.195552
O	0.426311	-1.456006	-0.118493
Si	1.726767	1.634091	0.121639
Si	1.993085	-1.386231	0.352293
O	2.460016	0.188355	0.390595
O	1.947436	2.499107	1.504483
H	1.746072	3.435591	1.470740
O	2.363688	2.410445	-1.179456
H	3.317295	2.406983	-1.276966
O	3.004898	-2.118720	-0.714416
H	2.848286	-3.044117	-0.909399
O	2.069053	-2.070965	1.845181
H	2.911721	-2.048565	2.301970
C	-1.686077	-0.449252	-2.206650
H	-1.690258	-1.519419	-2.465717
C	-2.633589	1.279839	0.455654
H	-2.854935	1.721706	-0.513980
H	-2.145904	1.910249	1.192002
C	-3.278197	0.127476	0.843521
H	-3.945590	-0.350596	0.132737
H	-2.063220	-1.219701	0.557347
H	-1.910877	0.187952	-3.061141
C	-3.440741	-0.272714	2.278776
H	-4.360773	0.193103	2.652836
H	-3.536524	-1.352714	2.397018
H	-2.612356	0.080419	2.896318

E_{SCF}= -1324,003855 au
G_{423}= -1323,902691 au
E_{disp}= -35,7462 kcal·mol^{-1}

30a

Ta	1.309599	-0.085311	-0.086818
O	0.251795	1.483451	-0.104930
O	0.125960	-1.563341	0.070832
Si	-1.396316	1.585425	0.026355
Si	-1.524109	-1.516740	0.126789
O	-1.995770	0.058489	0.092130
O	-2.066487	2.267295	-1.303849
H	-1.864647	3.185632	-1.491469
O	-1.694145	2.427183	1.397794
H	-2.588096	2.442087	1.743711
O	-2.116809	-2.117960	1.530318
H	-1.881206	-3.014541	1.775015
O	-2.044852	-2.333258	-1.194199
H	-2.986116	-2.359479	-1.374415
C	2.728999	-0.099964	1.206254
H	3.106868	-1.080387	1.522117
H	3.163576	0.722740	1.776458
C	2.364371	-0.258856	-1.953391
H	2.709271	0.773123	-2.146046
H	1.601061	-0.458067	-2.726909
C	3.539703	-1.226793	-2.121584
H	4.314099	-0.966882	-1.392725
H	3.217703	-2.245245	-1.869313
C	4.129579	-1.230291	-3.531789
H	4.496452	-0.235352	-3.805245
H	4.968318	-1.929453	-3.613177
H	3.379754	-1.521285	-4.274862

E_{SCF}= -1324,049352 au
G_{423}= -1323,947502 au
E_{disp}= -34,2636 kcal·mol^{-1}

31a

Ta	0.969038	-0.165133	0.042505
O	-0.223815	1.334137	-0.081137
O	-0.467790	-1.423611	0.070856
Si	-1.830959	1.619419	-0.067021
Si	-2.108860	-1.396049	-0.006473
O	-2.602877	0.165900	-0.041054
O	-2.353118	2.367451	-1.434742
H	-2.073486	3.273208	-1.577274
O	-2.164923	2.502939	1.276434
H	-3.084387	2.608970	1.526110
O	-2.806681	-2.063618	1.320523
H	-2.683525	-3.002963	1.466162
O	-2.512263	-2.196119	-1.384474
H	-3.420956	-2.139587	-1.685119
C	2.261762	0.470376	-1.570744
H	2.199092	-1.809263	0.165547
H	2.545780	1.473083	-1.191843
H	1.622688	0.677234	-2.443052
H	1.866948	-1.950086	-0.546545
C	1.976927	-0.131890	1.691227
H	1.814732	-0.513503	2.698161
C	3.521020	-0.282203	-2.013288
H	4.152050	-0.501246	-1.143307
H	3.236191	-1.256205	-2.429651
H	2.892731	0.474138	1.612741
C	4.347444	0.476055	-3.051361
H	5.231727	-0.094141	-3.354089
H	3.756464	0.680651	-3.949946
H	4.689373	1.438104	-2.656192

E_{SCF}= -1325,228056 au
G_{423}= -1325,109623 au
E_{disp}= -36,8477 kcal·mol^{-1}

TS(31a-26)

Ta	-0.750881	-0.512938	-0.303425
O	0.049824	1.238234	-0.320444
O	0.850091	-1.469464	0.115836

Si	1.561953	1.824645	-0.077036
Si	2.395655	-1.054272	0.477216
O	2.555444	0.570284	0.297929
O	1.632628	2.841260	1.212861
H	1.217493	3.700469	1.121529
O	2.017917	2.567507	-1.468038
H	2.949707	2.755554	-1.591818
O	3.481854	-1.724034	-0.554134
H	3.536211	-2.680562	-0.586222
O	2.646855	-1.515219	2.034036
H	3.463132	-1.242424	2.456560
C	-2.663728	0.405871	0.623380
H	-1.581682	-1.784887	0.848434
H	-2.595829	1.079190	-0.251322
H	-2.125457	-0.976396	0.853300
C	-1.484890	-1.107447	-1.978427
H	-1.203813	-2.088715	-2.376673
C	-4.104031	-0.092893	0.751393
H	-4.174983	-0.799425	1.589005
H	-4.357434	-0.665512	-0.147202
H	-2.024735	-0.500235	-2.708910
H	-2.368902	0.997423	1.499342
C	-5.115309	1.031960	0.959604
H	-6.131995	0.637665	1.050457
H	-4.894454	1.600121	1.868763
H	-5.103644	1.733666	0.119525

E_{SCF}= -1325,202971 au
G_{423}= -1325,084399 au
E_{disp}= -36,7375 kcal·mol^{-1}

TS(26-30b)

Ta	-0.996167	-0.499989	-0.244331
O	-0.115142	1.211438	-0.369591
O	0.590184	-1.478226	0.198556
Si	1.441278	1.723337	-0.327552
Si	2.158300	-1.115213	0.488846
O	2.394437	0.478269	0.159867
O	1.668209	2.918041	0.779893
H	1.391404	3.801931	0.533674
O	1.825704	2.234558	-1.842001
H	2.754665	2.278354	-2.074508
O	3.189985	-1.922062	-0.502773
H	3.153373	-2.879931	-0.495739
O	2.438623	-1.447037	2.074066
H	3.301816	-1.228671	2.429637
C	-1.726038	-1.171804	-1.889023
H	-1.624849	-2.267646	-1.933576
C	-2.827473	0.876287	0.547053
H	-3.084703	1.147650	-0.479880
C	-3.263063	-0.351705	0.992701
H	-3.840769	-1.010616	0.356859
H	-1.860147	-1.459313	1.022989
H	-2.043389	-0.742622	-2.838532
H	-3.300660	-0.568504	2.055812
C	-2.419170	1.986101	1.477872
H	-1.635144	2.605634	1.040444
H	-3.277440	2.630925	1.701742
H	-2.047785	1.593568	2.429654

E_{SCF}= -1324,000164 au
G_{423}= -1323,899887 au
E_{disp}= -36,6789 kcal·mol^{-1}

30b

Ta	1.261357	-0.037010	-0.176858
O	0.344516	1.590685	0.141489
O	-0.029298	-1.430932	-0.261805
Si	-1.289168	1.787759	0.325429
Si	-1.668090	-1.263061	-0.144804
O	-2.006141	0.327748	0.100367
O	-1.912456	2.769014	-0.829401
H	-1.656625	3.693032	-0.821278
O	-1.515349	2.362104	1.841457
H	-2.402271	2.361811	2.205363
O	-2.282342	-2.043943	1.157962
H	-2.110344	-2.982959	1.246993
O	-2.283236	-1.800433	-1.564430
H	-3.228814	-1.733924	-1.707793
C	2.716148	-0.407777	1.021649
H	3.023325	-1.455412	1.129757
H	3.231584	0.255826	1.718114
C	2.248466	0.073962	-2.094997
H	2.809221	1.021009	-1.991933
C	3.250698	-1.028698	-2.443117
H	4.062613	-1.069819	-1.714179
H	2.772260	-2.015033	-2.466320
H	3.687278	-0.868054	-3.439026
C	1.199065	0.254776	-3.206468
H	0.497049	1.071393	-3.002027
H	1.679909	0.484971	-4.166973
H	0.609369	-0.656408	-3.355461

E_{SCF}= -1324,046225 au
G_{423}= -1323,943972 au
E_{disp}= -36,3480 kcal·mol^{-1}

31b

Ta	0.932932	-0.155172	-0.028400
O	-0.248508	1.360823	-0.092091
O	-0.520307	-1.397411	-0.003254
Si	-1.847528	1.664670	0.025205
Si	-2.161450	-1.347387	0.012257
O	-2.636707	0.220739	0.047766
O	-2.434125	2.465865	-1.285654
H	-2.177217	3.383108	-1.393002
O	-2.095345	2.509251	1.412168
H	-2.996838	2.601826	1.724801
O	-2.795372	-2.042156	1.357978
H	-2.676659	-2.986489	1.471462
O	-2.654341	-2.104300	-1.361234
H	-3.579526	-2.032518	-1.602477
C	2.218054	0.500091	-1.644439
H	2.130281	-1.828523	0.029284
H	2.379896	1.523332	-1.240870
H	1.794233	-1.932537	-0.687075
C	1.956519	-0.182108	1.612197

H	1.774013	-0.580608	2.609366
C	3.593854	-0.150334	-1.820777
H	4.142715	-0.242841	-0.878756
H	3.505597	-1.154435	-2.250013
H	2.891860	0.395222	1.556369
H	4.218395	0.434676	-2.508740
C	1.486113	0.637326	-2.984499
H	0.545645	1.188005	-2.891243
H	2.103832	1.167039	-3.722293
H	1.254479	-0.345206	-3.411781

E_{SCF}= -1325,225190 au
G_{423}= -1325,106287 au
E_{disp}= -38,6914 kcal·mol^{-1}

TS(31b-26)

Ta	-0.905427	-0.455240	-0.279783
O	0.014050	1.231871	-0.411834
O	0.634940	-1.485126	0.204416
Si	1.572205	1.723432	-0.259847
Si	2.214778	-1.158336	0.491543
O	2.484331	0.435620	0.195269
O	1.749503	2.839050	0.934550
H	1.431900	3.726417	0.759677
O	2.035839	2.314995	-1.719517
H	2.975176	2.386305	-1.896858
O	3.219823	-1.970937	-0.520369
H	3.196808	-2.928984	-0.497048
O	2.487401	-1.527597	2.069113
H	3.340121	-1.297466	2.442123
C	-2.779619	0.609828	0.585479
H	-1.794672	-1.619037	0.953295
H	-2.582250	1.253733	-0.295383
H	-2.302336	-0.801285	0.883285
C	-1.661526	-1.108262	-1.922593
H	-1.451869	-2.130699	-2.255323
C	-4.231756	0.145306	0.502563
H	-4.473794	-0.545812	1.318843
H	-4.920588	0.994506	0.585986
H	-4.427472	-0.372883	-0.438441
H	-2.141317	-0.507324	-2.699229
C	-2.480657	1.391215	1.862420
H	-1.472868	1.815037	1.866433
H	-3.187912	2.219531	1.992848
H	-2.576014	0.747384	2.744803

E_{SCF}= -1325,202317 au
G_{423}= -1325,083093 au
E_{disp}= -38,6067 kcal·mol^{-1}

32

Ta	-1.246428	-0.147652	-0.151729
O	-0.056512	1.339598	-0.156995
O	0.116540	-1.469172	-0.012776
Si	1.565665	1.568863	-0.085817
Si	1.761980	-1.464847	0.082593
O	2.277273	0.089503	0.019808
O	2.029764	2.377740	1.264496
H	1.738612	3.285484	1.365785
O	1.995656	2.351121	-1.461234
H	2.929365	2.436334	-1.660874
O	2.456991	-2.226659	-1.192029
H	2.324319	-3.171985	-1.279065
O	2.129545	-2.177404	1.514471
H	3.032506	-2.117098	1.831083
H	-2.658490	-1.665957	0.027254
H	-2.252870	-1.800574	0.690567
C	-2.336249	-0.163683	-1.717894
H	-2.601034	-0.536371	-2.701327
H	-2.892734	0.763832	-1.441772
H	-2.317315	0.421640	1.147367

E_{SCF}= -1207,288260 au
G_{423}= -1207,242779 au
E_{disp}= -25,6826 kcal·mol^{-1}

TS(26-33)

Ta	1.321616	-0.000795	-0.070531
O	0.225567	1.527650	-0.029832
O	0.224985	-1.528990	0.000220
Si	-1.432344	1.552587	0.012591
Si	-1.433093	-1.553275	-0.006285
O	-1.968873	-0.000023	-0.021197
O	-2.068297	2.269531	-1.314863
H	-1.859642	3.191499	-1.474825
O	-1.833975	2.314181	1.404607
H	-2.751337	2.306376	1.682789
O	-2.038163	-2.215823	1.364021
H	-1.803034	-3.121987	1.570842
O	-1.868911	-2.368034	-1.356663
H	-2.797373	-2.400619	-1.593066
C	3.244818	0.007340	0.334027
H	3.863577	-0.889983	0.424135
H	2.791099	-0.001571	-1.159346
H	3.848213	0.915935	0.417851

E_{SCF}= -1206,075995 au
G_{423}= -1206,045879 au
E_{disp}= -23,2436 kcal·mol^{-1}

33

Ta	-1.306956	-0.000543	-0.038762
O	-0.215402	-1.511563	-0.023291
O	-0.214123	1.509880	-0.009943
Si	1.445937	-1.548078	0.014493
Si	1.447460	1.544791	-0.010515
O	1.999152	-0.001981	-0.004889
O	2.063511	-2.259464	-1.323594
H	1.849630	-3.179456	-1.487892
O	1.842366	-2.331336	1.394878
H	2.752289	-2.301481	1.694905
O	2.036545	2.231601	1.353617
H	1.806495	3.143980	1.537480
O	1.875257	2.351471	-1.367517
H	2.797617	2.354699	-1.628552
C	-3.421438	-0.002092	0.112137
H	-3.831913	0.887443	0.605223
H	-3.774679	-0.003723	-0.936295

H	-3.828373	-0.891964	0.607626

E_{SCF}= -1206,089021 au
G_{423}= -1206,058575 au
E_{disp}= -22,6752 kcal·mol^{-1}

TS(33-34)

Ta	1.210029	-0.066135	-0.179864
O	0.409625	1.651932	-0.301502
O	0.225316	-1.694651	-0.199494
Si	-1.207531	1.639228	0.081783
Si	-1.397802	-1.502572	0.083393
O	-1.777253	0.096337	-0.084680
O	-2.085677	2.510483	-0.992257
H	-1.902682	3.448838	-1.063855
O	-1.335440	2.202009	1.615412
H	-2.165540	2.079778	2.079314
O	-1.834138	-1.909509	1.611601
H	-1.659850	-2.803897	1.910062
O	-2.162254	-2.394993	-1.056507
H	-3.116781	-2.332679	-1.119887
C	2.851792	-0.104233	1.155412
H	2.420640	0.009923	2.164574
H	3.415871	-1.042581	1.126617
H	3.544133	0.727951	0.984988
H	0.269803	-0.080940	-2.211032
H	1.066053	-0.121556	-2.229708

E_{SCF}= -1207,248803 au
G_{423}= -1207,202204 au
E_{disp}= -26,1578 kcal·mol^{-1}

34

Ta	-1.344544	0.107936	-0.230567
O	-0.259902	-1.438054	-0.074451
O	-0.162810	1.554935	-0.083452
Si	1.378417	-1.536254	0.114557
Si	1.494801	1.556092	0.066193
O	1.979942	-0.004605	0.172688
O	2.111516	-2.241856	-1.167490
H	1.817498	-3.113943	-1.436660
O	1.620777	-2.331269	1.523671
H	2.518470	-2.445888	1.839933
O	1.965304	2.274185	1.458445
H	1.813673	3.215425	1.560566
O	2.057684	2.305917	-1.272771
H	2.994810	2.264079	-1.470505
C	-2.505781	-0.164618	1.559862
H	-1.825411	-0.420057	2.386357
H	-3.042542	0.754184	1.824877
H	-3.257159	-0.956502	1.472512
H	-1.641808	-0.241988	-1.922116
H	-3.006475	0.453789	-0.704802

E_{SCF}= -1207,321933 au
G_{423}= -1207,273989 au
E_{disp}= -25,5422 kcal·mol^{-1}

35

Ta	1.365524	-0.104601	-0.226285
O	0.059104	-1.434998	-0.052103
O	0.210613	1.427467	-0.068058
Si	-1.597366	-1.453287	0.061719
Si	-1.413955	1.601048	0.073855
O	-2.095436	0.101820	0.145988
O	-2.086207	-2.173401	1.447944
H	-1.982795	-3.123300	1.526487
O	-2.132992	-2.222808	-1.279234
H	-3.050747	-2.119424	-1.536016
O	-2.100082	2.313562	-1.235074
H	-1.766864	3.171144	-1.504715
O	-1.666004	2.438551	1.460318
H	-2.569948	2.598305	1.736603
C	2.539471	-0.012486	1.584457
H	1.950791	0.510017	2.351503
H	2.563531	-1.078103	1.867822
H	1.559990	0.316622	-1.919406
H	2.841383	-0.859294	-0.900814
H	2.625662	1.389081	-1.030120
H	2.899435	1.400745	-0.301029
H	3.565656	0.350842	1.616207

E_{SCF}= -1208,502615 au
G_{423}= -1208,439769 au
E_{disp}= -27,7566 kcal·mol^{-1}

TS(35-1b)

Ta	-1.335872	-0.314964	-0.213931
O	-0.331332	1.320084	-0.158215
O	0.137057	-1.491416	-0.034869
Si	1.264415	1.690874	-0.045245
Si	1.764010	-1.311737	0.167861
O	2.110997	0.288790	0.100203
O	1.602900	2.544563	1.316402
H	1.277852	3.444834	1.370354
O	1.661410	2.508176	-1.409259
H	2.590379	2.626616	-1.613807
O	2.615591	-2.013831	-1.041691
H	2.540049	-2.962444	-1.157790
O	2.103680	-1.949157	1.640480
H	2.981724	-1.816433	2.001956
C	-2.812180	0.850939	1.159885
H	-1.466864	-0.343232	-1.944867
H	-2.936293	-0.819224	-0.792008
H	-2.126668	-1.481516	1.037253
H	-2.972546	1.558652	0.334494
H	-2.253255	1.353067	1.953297
H	-2.525639	-0.607912	1.198223
H	-3.804369	0.579563	1.528044

E_{SCF}= -1208,477951 au
G_{423}= -1208,412310 au
E_{disp}= -27,9038 kcal·mol^{-1}

TS(34-1a)

Ta	1.287969	-0.011755	-0.226971
O	0.169833	1.493993	-0.112082
O	0.138580	-1.491062	-0.092161
Si	-1.467389	1.558507	0.121644

Si	-1.505507	-1.523126	0.101722
O	-2.043210	0.023772	0.224213
O	-2.244299	2.238149	-1.151077
H	-1.982029	3.118985	-1.423759
O	-1.689319	2.390150	1.515848
H	-2.580550	2.468971	1.860185
O	-1.935065	-2.256043	1.503725
H	-1.781867	-3.199231	1.580816
O	-2.109083	-2.288821	-1.214385
H	-3.046575	-2.208588	-1.397358
C	3.297937	-0.015220	1.180638
H	3.063591	-0.894132	1.781159
H	4.382765	-0.021730	0.988993
H	3.070391	0.879738	1.760019
H	2.420325	-0.027054	-1.580719
H	3.116667	-0.027912	-0.062963

E_{SCF}= -1207,258273 au
G_{423}= -1207,209143 au
E_{disp}= -24,7210 kcal·mol^{-1}

TS(26-36a)

Ta	0.995503	-0.638597	-0.003629
O	0.301966	1.135842	0.085214
O	-0.759748	-1.417933	0.023852
Si	-1.169213	1.869726	0.141434
Si	-2.312731	-0.921136	-0.128790
O	-2.326195	0.719843	-0.006136
O	-1.397328	2.896809	-1.118839
H	-0.858946	3.689173	-1.152485
O	-1.234179	2.642932	1.588319
H	-2.077672	3.000110	1.871259
O	-3.268538	-1.455824	1.094502
H	-3.375703	-2.403333	1.193012
O	-2.844929	-1.423347	-1.598188
H	-3.710095	-1.130843	-1.889849
C	2.918803	0.430513	-0.948453
H	2.267001	0.758926	-1.767941
H	3.696879	-0.168317	-1.431401
H	2.848271	-0.531586	0.150873
C	2.246897	-1.315362	1.325943
H	2.259755	-2.383557	1.028798
C	3.510450	1.641796	-0.226698
H	4.195372	1.337310	0.572472
H	4.075837	2.279262	-0.914312
H	2.727755	2.254905	0.227176
H	2.856335	-1.113036	2.200243
H	1.345443	-1.579984	-1.454498

E_{SCF}= -1285,900029 au
G_{423}= -1285,804265 au
E_{disp}= -34,088800 kcal·mol^{-1}

36a

Ta	1.088226	-0.531468	-0.008036
O	0.223936	1.147868	0.191479
O	-0.632124	-1.396836	-0.025386
Si	-1.284083	1.804138	0.214407
Si	-2.215565	-1.032214	-0.207399
O	-2.365876	0.594660	-0.007493
O	-1.533753	2.860240	-1.016763
H	-1.032837	3.677505	-1.016976
O	-1.435267	2.520496	1.683965
H	-2.298620	2.851988	1.936675
O	-3.148629	-1.712716	0.959781
H	-3.275533	-2.662351	0.929103
O	-2.674398	-1.498644	-1.713311
H	-3.515307	-1.182638	-2.048277
C	2.662398	0.408997	-1.154753
H	2.388685	0.581297	-2.201358
H	3.443042	-0.372627	-1.196852
H	3.006435	-0.701166	1.926285
C	2.116531	-1.293551	1.682148
H	2.453334	-2.305015	1.399879
C	3.222555	1.688914	-0.516120
H	3.489876	1.557444	0.539441
H	4.131409	2.029894	-1.026491
H	2.490997	2.499895	-0.558073
H	1.500574	-1.384321	2.582896
H	1.292516	-1.546353	-1.423589

E_{SCF}= -1285,952907 au
G_{423}= -1285,857133 au
E_{disp}= -33,312500 kcal·mol^{-1}

36b

Ta	-1.110949	-0.178157	-0.317797
O	0.380148	-1.398807	-0.141471
O	0.015432	1.276373	0.125079
Si	2.002589	-1.361141	0.038071
Si	1.619408	1.622715	0.283377
O	2.438072	0.206067	0.299672
O	2.833184	-1.813087	-1.306625
H	2.628905	-2.667884	-1.689699
O	2.354167	-2.310471	1.330341
H	3.274301	-2.401172	1.583327
O	1.936739	2.360410	1.713002
H	1.650592	3.269151	1.818691
O	2.019727	2.562930	-1.001351
H	2.949079	2.676533	-1.207844
H	-2.974924	-1.666434	0.473836
C	-2.475647	-0.913611	1.122772
H	-1.914830	-1.498937	1.864419
C	-3.508819	-0.009291	1.798827
H	-4.106669	0.542373	1.069089
H	-4.200188	-0.587722	2.420848
H	-3.023950	0.723435	2.450388
C	-2.423616	1.078214	-1.483550
H	-3.327328	0.546404	-1.808768
H	-2.727277	1.911237	-0.826252
H	-1.969860	1.517209	-2.378034
H	-1.237800	-1.019962	-1.848532

E_{SCF}= -1285,953759 au
G_{423}= -1285,858312 au
E_{disp}= -32,9694 kcal·mol^{-1}

36c

Ta	-1.144857	-0.147777	-0.126541

O	0.256523	-1.388828	0.101374
O	0.090243	1.349600	-0.076980
Si	1.901706	-1.406176	0.214401
Si	1.702816	1.594038	-0.148881
O	2.436868	0.129615	0.035418
O	2.596538	-2.274033	-0.990607
H	2.429055	-3.217437	-1.020951
O	2.236799	-2.018421	1.699798
H	3.140461	-1.968571	2.016067
O	2.252515	2.515831	1.096083
H	2.034841	3.449213	1.085086
O	2.057486	2.260279	-1.607286
H	2.972210	2.256210	-1.894181
C	-2.578769	-1.566754	-0.940324
H	-2.204457	-2.084335	-1.831115
H	-3.559382	-1.152373	-1.201138
H	-3.067518	-0.290749	1.843512
C	-2.401508	0.488965	1.469748
H	-1.882999	0.963297	2.303506
H	-1.437833	0.471229	-1.730716
C	-3.069078	1.461774	0.512164
H	-2.670922	1.382321	-0.551013
H	-4.136683	1.280897	0.383380
H	-2.890566	2.506469	0.767587
H	-2.734621	-2.334750	-0.161720

E_{SCF}= -1285,957218 au
G_{423}= -1285,858279 au
E_{disp}= -34,011400 kcal·mol^{-1}

TS(36b-37)

Ta	-0.928015	-0.646496	0.025586
O	-0.184035	1.116313	-0.016463
O	0.847496	-1.418083	0.037426
Si	1.283279	1.848359	-0.057911
Si	2.406086	-0.946767	0.124437
O	2.444559	0.696257	0.040318
O	1.531687	2.838363	1.229771
H	0.952467	3.596226	1.324865
O	1.340631	2.668256	-1.481518
H	2.177210	3.060535	-1.737276
O	3.311122	-1.464483	-1.147578
H	3.408357	-2.411041	-1.262983
O	3.002984	-1.493055	1.556066
H	3.890270	-1.224655	1.800725
H	-2.670208	-0.035734	-0.321170
C	-2.055210	-0.900997	-1.578598
H	-1.912351	-0.122737	-2.340679
C	-3.020706	-1.981821	-1.998635
H	-3.187221	-2.727103	-1.216484
H	-3.996453	-1.569832	-2.282572
H	-2.628324	-2.508126	-2.876241
C	-1.602205	-1.967169	1.586362
H	-2.689214	-1.963939	1.726999
H	-1.293140	-2.980913	1.284061
H	-1.138782	-1.770016	2.559679
H	-2.453194	0.292156	0.624783

E_{SCF}= -1285,918597 au
G_{423}= -1285,825986 au
E_{disp}= -33,480100 kcal·mol^{-1}

37

Ta	-1.127604	-0.161468	-0.237149
O	0.319961	-1.416129	-0.197846
O	0.054492	1.338524	0.008674
Si	1.939750	-1.390907	0.067633
Si	1.651874	1.619444	0.175566
O	2.428691	0.168495	0.184654
O	2.785840	-2.030299	-1.187518
H	2.693717	-2.970428	-1.349985
O	2.190036	-2.227023	1.460719
H	3.058864	-2.175230	1.862825
O	2.043928	2.322627	1.609903
H	1.636265	3.166024	1.813283
O	2.113352	2.545197	-1.101833
H	3.041706	2.772895	-1.175084
H	-2.316472	-1.794605	-0.473226
C	-2.275342	-0.390628	1.316272
H	-1.824098	-1.036648	2.084208
C	-3.592827	0.210510	1.732163
H	-4.033290	0.842762	0.955722
H	-4.327696	-0.566688	1.977221
H	-3.473006	0.828096	2.631313
C	-2.240619	0.691645	-1.877424
H	-3.177765	0.166860	-2.098732
H	-2.496685	1.719663	-1.576837
H	-1.668775	0.766948	-2.809708
H	-1.918067	-1.812273	-1.174033

E_{SCF}= -1285,922835 au
G_{423}= -1285,828975 au
E_{disp}= -33,369200 kcal·mol^{-1}

TS(36a-16)

Ta	0.993799	-0.042330	-0.096791
O	-0.476311	1.236183	0.263100
O	-0.367078	-1.347283	-0.294527
Si	-2.088038	1.290232	0.405936
Si	-1.981111	-1.643620	-0.281180
O	-2.695438	-0.197697	0.035292
O	-2.828443	2.312981	-0.654511
H	-2.668822	3.251179	-0.540340
O	-2.430129	1.705785	1.965532
H	-3.351342	1.699667	2.231410
O	-2.262396	-2.764033	0.877745
H	-3.010022	-3.349543	0.748535
O	-2.565468	-2.256904	-1.687459
H	-2.762287	-1.645848	-2.399437
C	1.705912	1.444552	-1.497060
H	1.468874	1.143793	-2.523394
H	2.793626	1.242145	-1.409075
H	1.951192	1.847109	1.399422
C	1.841130	0.870139	1.883929
H	2.711303	0.723242	2.531868
C	1.405245	2.928787	-1.293591
H	1.670101	3.285592	-0.293064

H	1.954808	3.547798	-2.013242
H	0.339135	3.125108	-1.426713
H	0.940121	0.885191	2.500295
H	1.750466	-0.869559	-1.447905
C	4.042915	-1.505683	0.242597
H	4.557743	-0.651961	0.698928
H	4.619584	-2.399795	0.503694
H	4.093120	-1.376379	-0.840764
C	2.594744	-1.618034	0.714730
H	2.566785	-1.931270	1.769838
H	2.198178	-0.315632	1.310861
H	2.060603	-2.404129	0.173232

E_{SCF}= -1365,711528 au
G_{423}= -1365,549960 au
E_{disp}= -45,522800 kcal·mol^{-1}

TS(36c-6)

Ta	-1.135546	-0.019410	-0.143135
O	0.193011	-1.369876	0.093283
O	0.172847	1.389495	-0.090022
Si	1.824995	-1.458445	0.260583
Si	1.801621	1.539911	-0.138683
O	2.452142	0.045622	0.083821
O	2.522397	-2.369501	-0.914407
H	2.316437	-3.305506	-0.932753
O	2.096217	-2.072575	1.759756
H	2.993317	-2.052220	2.097214
O	2.387053	2.454941	1.094138
H	2.123096	3.375863	1.126438
O	2.194096	2.161781	-1.607163
H	3.122539	2.213180	-1.840540
C	-2.438404	-1.830282	-0.989942
H	-1.823943	-1.873260	-1.895036
H	-3.477896	-1.834914	-1.328807
H	-2.798457	-0.854703	0.012195
C	-2.581701	0.194562	1.157630
H	-2.946745	-0.311665	2.048409
H	-1.718879	0.617390	-1.685422
C	-3.216940	1.537361	0.828737
H	-2.741658	2.033197	-0.036223
H	-4.277548	1.451664	0.567651
H	-3.117304	2.221671	1.677485
H	-2.250566	-2.733223	-0.402157

E_{SCF}= -1285,901998 au
G_{423}= -1285,806924 au
E_{disp}= -34,072700 kcal·mol^{-1}

VII. Production of propane and methane from Ta-alkyl-alkylidene 14

TS(30a-38a)

Ta	0.758762	-0.288171	-0.374524
O	-0.703875	-1.373203	0.216465
O	-0.432074	1.224571	-0.513365
Si	-2.311182	-1.258849	0.519109
Si	-1.971660	1.649239	-0.172821
O	-2.772772	0.302346	0.324851
O	-2.682649	-1.638860	2.074258
H	-2.557873	-2.548526	2.349537
O	-3.052380	-2.263842	-0.549287
H	-4.005087	-2.200938	-0.635756
O	-2.797232	2.183451	-1.489962
H	-2.455798	2.954580	-1.945571
O	-1.906243	2.788799	1.010855
H	-2.734713	3.098904	1.380519
C	1.983361	-2.176674	0.535414
H	1.697293	-1.836771	1.538441
H	2.032525	-1.593006	-0.802584
C	1.659445	-0.786696	-2.046146
H	2.496209	-0.103120	-2.253385
C	2.141757	0.865050	0.826117
H	1.793080	0.837395	1.870238
H	3.106236	0.335935	0.822330
H	1.368838	-3.058856	0.330254
H	1.513548	-1.521022	-2.835194
C	3.471579	-2.527152	0.526197
H	3.790809	-2.906225	-0.451297
H	4.093788	-1.655650	0.752439
H	3.708002	-3.295827	1.268830
C	2.354086	2.321738	0.386739
H	1.408988	2.864455	0.478305
H	2.619317	2.363033	-0.678669
C	3.441071	3.035798	1.190223
H	3.564070	4.073017	0.861523
H	3.191936	3.050407	2.256232
H	4.409004	2.534759	1.084214

E_{SCF}= -1403,838782 au
G_{423}= -1403,671082 au
E_{disp}= -46,409 kcal·mol^{-1}

38a

Ta	-0.775892	-0.474838	-0.044294
O	0.840670	-1.151355	-0.734044
O	0.148390	1.064632	0.741794
Si	2.448062	-0.780939	-0.771164
Si	1.645310	1.711852	0.748153
O	2.651023	0.664853	-0.034894
O	2.996840	-0.597401	-2.305354
H	3.018166	-1.371645	-2.870379
O	3.203707	-2.002595	0.021817
H	4.129410	-1.892843	0.245960
O	2.282956	1.864387	2.255961
H	1.858361	2.479276	2.856431
O	1.563084	3.154099	-0.036375
H	2.386334	3.598505	-0.246279
C	-2.056106	-2.013480	-0.936329
H	-3.128334	-1.914242	-0.725390
C	-1.922233	0.945190	-1.196709
H	-1.229423	1.731574	-1.525407
H	-2.322128	0.463505	-2.096219

H	-1.747890	-3.012003	-0.592484
C	-3.064108	1.576702	-0.384746
H	-2.665507	2.020020	0.536264
H	-3.776321	0.801743	-0.074049
C	-1.513912	-1.041770	1.894620
H	-0.890221	-0.508095	2.623088
H	-2.496547	-0.536257	1.920419
H	-1.946365	-2.014184	-2.030713
C	-1.661828	-2.508224	2.303982
H	-2.371258	-3.038035	1.665040
H	-0.706869	-3.040605	2.247361
H	-2.015698	-2.596894	3.337528
C	-3.819053	2.656174	-1.162777
H	-4.627203	3.088325	-0.563735
H	-3.145413	3.467321	-1.455364
H	-4.260112	2.244425	-2.075917

E_{SCF}= -1403,889818 au
G_{423}= -1403,720609 au
E_{disp}= -45,9427 kcal·mol^{-1}

TS(38a-13)

Ta	0.594023	-0.747575	-0.115310
O	0.111108	1.097244	0.096790
O	-1.283007	-1.227779	-0.075840
Si	-1.223120	2.029875	0.290962
Si	-2.755452	-0.528252	-0.095813
O	-2.555973	1.088628	0.139582
O	-1.358072	3.179502	-0.876696
H	-0.704392	3.880468	-0.884339
O	-1.099974	2.697444	1.789056
H	-1.866879	3.156035	2.136494
O	-3.724159	-1.026476	1.136439
H	-3.951627	-1.957079	1.168293
O	-3.428786	-0.844456	-1.563246
H	-4.265831	-0.424707	-1.769132
C	2.672654	0.259199	-0.822518
H	2.129626	0.688646	-1.674891
H	3.446665	-0.378526	-1.265352
H	2.417238	-0.735684	0.245804
C	1.669804	-1.605950	1.259448
H	1.665193	-2.589683	0.728006
C	0.854327	-1.895572	-1.936231
H	0.337374	-2.857908	-1.822939
H	0.372750	-1.377632	-2.775087
H	1.894554	-2.094077	-2.210999
C	2.346484	-1.626957	2.594986
H	1.813446	-2.292022	3.283201
H	3.382354	-1.981828	2.537693
H	2.355412	-0.631410	3.045142
C	3.301938	1.385548	-0.000771
H	2.507267	1.978625	0.463047
H	3.883680	0.958037	0.826584
C	4.206411	2.298872	-0.826001
H	3.646420	2.781494	-1.633768
H	4.648678	3.087674	-0.208819
H	5.025567	1.736116	-1.285520

E_{SCF}= -1403,846048 au
G_{423}= -1403,677675 au
E_{disp}= -46,108 kcal·mol^{-1}

VIII. Hydrogenolysis of ethane by 1b

TS(3a-26)

Ta	1.227304	0.314504	-0.132011
O	0.199790	-1.286515	0.035744
O	-0.353862	1.422442	-0.028052
Si	-1.383602	-1.728540	0.020292
Si	-1.971118	1.241871	0.046993
O	-2.297707	-0.372395	0.099852
O	-1.775258	-2.628504	1.336230
H	-1.449583	-3.529220	1.370153
O	-1.630609	-2.554625	-1.379775
H	-2.534709	-2.665933	-1.678996
O	-2.758018	1.792223	-1.289015
H	-2.630108	2.711183	-1.530144
O	-2.484743	2.000682	1.410971
H	-3.418317	1.950238	1.622648
C	2.612910	0.457396	1.260751
H	3.248607	1.350648	1.188546
H	2.883240	-0.177018	2.103715
C	3.567346	-0.876835	-0.396752
H	4.319793	-0.594153	0.335707
H	3.306455	-1.925194	-0.265825
H	3.982458	-0.685690	-1.384649
H	1.780614	1.323443	-1.491539
H	2.197592	-0.635311	-1.245803

E_{SCF}= -1246,538636 au
G_{423}= -1246,468750 au
E_{disp}= -29,7295 kcal·mol^{-1}

39

Ta	1.313283	-0.035458	-0.012825
O	0.093490	1.431998	0.177670
O	-0.100060	-1.293539	-0.259024
Si	-1.517775	1.679784	0.267507
Si	-1.742620	-1.279217	-0.332414
O	-2.265275	0.240750	-0.015220
O	-2.069041	2.695656	-0.901017
H	-1.791984	3.612351	-0.858849
O	-1.846660	2.244006	1.773930
H	-2.765344	2.298933	2.042222
O	-2.423482	-2.242332	0.807937
H	-2.292366	-3.188752	0.731677
O	-2.131022	-1.755307	-1.856748
H	-3.036589	-1.633657	-2.147412
C	2.611057	0.893867	-1.468886
H	2.571442	-1.665468	-0.232185
H	2.823147	1.910685	-1.105134
H	2.138202	0.997298	-2.452847
H	2.243108	-1.665530	-0.955913

H	3.573094	0.387761	-1.606342
C	2.309996	-0.313922	1.614167
H	2.189973	-0.887316	2.531170
H	3.195288	0.342868	1.636184

E_{SCF}= -1246,613112 au
G_{423}= -1246,544217 au
E_{disp}= -29,7072 kcal·mol^{-1}

TS(39-26)

Ta	1.261307	-0.222776	0.030957
O	0.164205	1.360428	0.087494
O	-0.167529	-1.482484	-0.009884
Si	-1.449470	1.645073	0.096666
Si	-1.804671	-1.378277	-0.116588
O	-2.231049	0.202275	-0.007378
O	-1.940250	2.500769	-1.218326
H	-1.674946	3.420290	-1.273024
O	-1.793012	2.423812	1.499783
H	-2.711220	2.481369	1.769027
O	-2.558518	-2.133496	1.128486
H	-2.427202	-3.078215	1.224588
O	-2.209291	-2.015559	-1.575132
H	-3.116426	-1.923326	-1.871521
C	2.718352	0.968977	-1.334208
H	2.150773	-1.400789	-1.158425
H	2.853229	1.686056	-0.511955
H	2.135404	1.441235	-2.129338
H	2.514887	-0.496934	-1.333530
H	3.719594	0.747945	-1.712050
C	2.369051	-0.493936	1.577053
H	2.364905	-1.446753	2.116265
H	2.902805	0.291057	2.118908

E_{SCF}= -1246,585080 au
G_{423}= -1246,515793 au
E_{disp}= -29,8299 kcal·mol^{-1}

TS(39-40)

Ta	-1.310012	-0.075249	-0.009000
O	-0.004995	1.342366	-0.126387
O	0.080031	-1.378483	0.044759
Si	1.613280	1.550293	-0.160492
Si	1.719077	-1.453038	0.133252
O	2.311422	0.064423	-0.043312
O	2.184249	2.399330	1.126996
H	1.921862	3.317972	1.205205
O	1.980458	2.281564	-1.584626
H	2.906308	2.369442	-1.817068
O	2.360783	-2.340936	-1.088258
H	2.208315	-3.287225	-1.079664
O	2.076187	-2.083199	1.608184
H	2.981008	-2.015968	1.918136
C	-2.425488	0.951302	1.519931
H	-2.690318	-1.349306	-0.234104
H	-2.546779	1.991797	1.180300
H	-1.897231	0.983747	2.479864
H	-2.328755	-1.511668	0.699838
H	-3.420786	0.530856	1.700408
C	-2.504835	-0.393015	-1.540337
H	-2.372834	-1.053199	-2.397760
H	-3.439370	0.177937	-1.595427

E_{SCF}= -1246,608118 au
G_{423}= -1246,539046 au
E_{disp}= -29,7315 kcal·mol^{-1}

40

Ta	-1.28051	-0.18718	-0.00462
O	-0.23154	1.41717	0.04444
O	0.05178	-1.50547	-0.05642
Si	1.39497	1.64231	0.01785
Si	1.71057	-1.41925	-0.01940
O	2.12302	0.16344	-0.00956
O	1.95091	2.36391	1.38168
H	1.62375	3.24070	1.59034
O	1.72989	2.49585	-1.34021
H	2.64858	2.62687	-1.58103
O	2.37561	-2.06091	-1.36978
H	2.28324	-3.00332	-1.52006
O	2.15777	-2.19777	1.34906
H	3.06444	-2.11831	1.65036
C	-2.05588	0.20312	1.96450
H	-2.44151	-0.56070	-2.45706
H	-2.90150	0.90071	1.92993
H	-1.27725	0.63135	2.60930
H	-2.92484	-0.87879	-0.02158
H	-2.42672	-0.72134	2.42179
C	-2.06344	0.32836	-1.93956
H	-1.28633	0.79986	-2.55501
H	-2.90540	1.02574	-1.85123

E_{SCF}= -1246,645081 au
G_{423}= -1246,572443 au
E_{disp}= -29,6679 kcal·mol^{-1}

41

Ta	1.339414	-0.072037	-0.361148
O	0.045757	-1.417883	-0.200853
O	0.233107	1.489198	-0.144323
Si	-1.598445	-1.402400	0.020807
Si	-1.373035	1.654218	0.145352
O	-2.063360	0.157738	0.182571
O	-2.025273	-2.156664	1.409247
H	-1.890364	-3.103735	1.472749
O	-2.228452	-2.112806	-1.312936
H	-3.168968	-2.028857	-1.478660
O	-2.148031	2.448514	-1.063527
H	-1.881790	3.351086	-1.247097
O	-1.512490	2.409402	1.594100
H	-2.384008	2.479979	1.987288
C	2.297254	0.005814	1.588490
H	1.627893	0.527146	2.287335
H	2.327283	-1.053432	1.887774
H	2.983919	-0.699775	-0.625526
H	2.747844	1.618133	-0.911851
H	2.827865	1.635456	-0.155262
H	3.310086	0.390393	1.710473

C	1.681261	0.122802	-2.499503
H	0.840256	0.674775	-2.942913
H	2.616192	0.514614	-2.900931
H	1.605432	-0.920215	-2.844888

E_{SCF}= -1247,819802 au
G_{423}= -1247,733878 au
E_{disp}= -32,4012 kcal·mol^{-1}

TS(41-34)

Ta	1.282663	-0.257929	0.004428
O	0.227953	1.352212	0.076744
O	-0.174540	-1.478199	-0.100558
Si	-1.379373	1.669454	0.112156
Si	-1.811358	-1.336401	-0.171135
O	-2.198492	0.248804	-0.006222
O	-1.871152	2.559552	-1.178600
H	-1.548120	3.459600	-1.246573
O	-1.677997	2.425354	1.537958
H	-2.591995	2.549694	1.799141
O	-2.550437	-2.111177	1.070581
H	-2.458770	-3.063982	1.123479
O	-2.258289	-1.925266	-1.636518
H	-3.163855	-1.790776	-1.921272
C	2.477647	1.024662	-1.544775
H	2.991002	-0.700525	0.208897
H	1.876918	-1.327115	-1.432597
H	2.739540	1.716064	-0.732753
H	1.788678	1.530273	-2.225456
H	2.205111	-0.436897	-1.618107
H	3.410592	0.794155	-2.064728
C	1.641028	-0.371886	2.115722
H	2.006480	-1.355793	2.424505
H	2.382020	0.368175	2.436938
H	0.694125	-0.161809	2.631744

E_{SCF}= -1247,800818 au
G_{423}= -1247,710369 au
E_{disp}= -32,4567 kcal·mol^{-1}

IX. Production of propane and methane from Ta-alkyl 19

TS(19-42)

Ta	-0.978400	0.165593	-0.034009
O	0.420993	1.518325	0.453041
O	0.323813	-1.149978	-0.405446
Si	2.028519	1.582773	0.420004
Si	1.961353	-1.314240	-0.525275
O	2.619966	0.122015	-0.097850
O	2.726947	1.773106	1.908465
H	2.463473	2.548658	2.406626
O	2.503539	2.786308	-0.601215
H	3.446854	2.929573	-0.694079
O	2.264131	-1.745914	-2.074345
H	3.088522	-2.201665	-2.250619
O	2.559799	-2.499096	0.445310
H	2.862500	-2.236043	1.316397
C	-2.621985	-0.143155	-1.167103
H	-2.431073	-0.975589	-1.866786
C	-1.871439	0.275160	1.915422
H	-1.137183	0.196006	2.717631
H	-2.574866	1.095952	2.072002
H	-1.399851	1.219818	-1.433367
C	-2.390765	-0.964095	1.333580
H	-1.916706	-1.904691	1.612371
H	-3.453188	-1.071526	1.146377
C	-3.959605	0.474438	-1.377476
H	-4.148264	1.328871	-0.723856
H	-4.085683	0.794378	-2.418488
H	-4.733388	-0.282957	-1.199355

E_{SCF}= -1323,989441 au
G_{423}= -1323,888113 au
E_{disp}= -36,1775 kcal·mol^{-1}

42

Ta	-0.976847	-0.318206	-0.143996
O	0.595200	-1.442907	0.018565
O	0.137412	1.207435	-0.387272
Si	2.190198	-1.266780	0.301449
Si	1.688986	1.696223	-0.149388
O	2.558056	0.332694	0.159134
O	3.113433	-2.017552	-0.837198
H	3.060856	-2.973597	-0.884695
O	2.513889	-1.825943	1.812011
H	3.399808	-1.701831	2.156628
O	1.696049	2.752986	1.097836
H	2.430660	3.365431	1.159028
O	2.329581	2.468010	-1.449894
H	2.716216	1.929189	-2.142277
C	-2.641793	0.759766	0.565718
H	-2.490646	1.759314	0.125405
C	-2.392109	-0.774017	-1.597355
H	-2.407775	-0.238636	-2.547195
H	-2.587890	-1.836633	-1.758034
H	-1.433928	-1.222857	1.289677
C	-3.369314	-0.138353	-0.520872
H	-4.080569	0.490946	-1.057993
H	-3.914099	-0.927077	-0.000359
C	-3.364299	0.847016	1.888527
H	-3.466705	-0.144534	2.338667
H	-2.801098	1.469669	2.589032
H	-4.367464	1.283206	1.793371

E_{SCF}= -1324,044033 au
G_{423}= -1323,936722 au
E_{disp}= -35,8867 kcal·mol^{-1}

TS(42-43)

Ta	0.986236	-0.291365	-0.195460
O	-0.546924	-1.435837	-0.048220
O	-0.143061	1.263174	0.048303

Si	-2.184595	-1.347600	0.073645
Si	-1.730732	1.662695	0.192636
O	-2.542564	0.234504	0.339777
O	-2.708371	-2.318341	1.292174
H	-2.089553	-2.526151	1.993627
O	-2.973601	-1.786426	-1.289966
H	-3.120814	-2.722274	-1.435388
O	-2.126695	2.504172	-1.151549
H	-2.976433	2.947066	-1.173483
O	-2.076993	2.589116	1.503471
H	-2.302920	2.140593	2.319689
C	2.578208	0.336071	0.992399
H	2.429384	1.244850	1.576439
H	1.984424	-1.819049	-0.393992
C	3.178123	0.637276	-0.443866
H	3.514914	1.673086	-0.447931
H	4.007943	-0.043966	-0.617180
C	2.186764	0.477448	-1.704285
H	1.810335	1.469479	-1.977592
H	3.165885	-0.401256	1.533418
C	2.799807	-0.235837	-2.892736
H	2.065012	-0.332518	-3.696673
H	3.655899	0.318392	-3.296926
H	3.134536	-1.238637	-2.618986

E_{SCF}= -1324,037195 au
G_{423}= -1323,928462 au
E_{disp}= -36,1194 kcal·mol^{-1}

43

Ta	-1.020140	-0.027498	-0.237705
O	0.336590	-1.417836	-0.053521
O	0.270783	1.331870	-0.046092
Si	1.960761	-1.495012	0.018451
Si	1.889906	1.545266	0.184071
O	2.544338	0.039227	0.181387
O	2.660338	-2.049302	-1.367050
H	2.352528	-2.890879	-1.708067
O	2.351173	-2.425396	1.314992
H	3.281246	-2.586183	1.482102
O	2.067996	2.325900	1.608354
H	2.866066	2.840830	1.736191
O	2.603743	2.464700	-0.971667
H	2.872299	2.036157	-1.786351
C	-2.673870	1.169077	-0.909709
H	-3.391247	0.803633	-1.642603
C	-2.475487	-0.310360	1.212401
H	-2.389992	-0.288425	2.293541
C	-3.167139	0.942194	0.570114
H	-4.248913	0.770046	0.559508
H	-2.963256	1.814317	1.194665
C	-2.948569	-1.609001	0.591399
H	-2.509675	-1.777985	-0.433997
H	-2.644039	-2.471986	1.184353
H	-4.027553	-1.640236	0.402148
H	-2.451633	2.219093	-1.107402
H	-1.274248	-0.829362	-1.773392

E_{SCF}= -1324,046676 au
G_{423}= -1323,938347 au
E_{disp}= -36,9944 kcal·mol^{-1}

TS(43-44)

Ta	1.102227	-0.185410	-0.234432
O	-0.162155	1.387246	-0.141052
O	-0.360676	-1.369110	-0.059829
Si	-1.752903	1.611446	-0.059943
Si	-1.983519	-1.403806	0.217659
O	-2.501087	0.149745	0.158761
O	-2.437489	2.192655	-1.450126
H	-2.057439	2.994709	-1.812164
O	-2.076263	2.616951	1.207934
H	-2.992556	2.866810	1.338822
O	-2.191658	-2.106446	1.681585
H	-3.046735	-2.497717	1.866338
O	-2.811996	-2.303233	-0.879866
H	-3.102141	-1.860542	-1.679504
C	2.360796	-1.207399	-1.416818
H	3.228559	-0.947099	-2.025440
C	2.243525	0.733487	1.397883
H	1.540947	1.174118	2.098635
C	2.598310	-0.637447	1.487070
H	3.569819	-0.991417	1.167151
H	2.122652	-1.239902	2.256851
C	2.865075	1.607442	0.372585
H	2.457135	1.407519	-0.696038
H	2.626753	2.659170	0.520997
H	3.939801	1.457474	0.245257
H	2.029470	-2.233193	-1.645320
H	1.455420	0.319074	-1.913618

E_{SCF}= -1323,990167 au
G_{423}= -1323,887085 au
E_{disp}= -37,6227 kcal·mol^{-1}

44

Ta	1.044919	-0.308656	-0.274926
O	-0.007764	1.324503	-0.337886
O	-0.458429	-1.428970	-0.090106
Si	-1.562835	1.711407	-0.048069
Si	-2.066539	-1.291521	0.262429
O	-2.405166	0.314789	0.198574
O	-2.292282	2.415923	-1.344900
H	-1.962985	3.271276	-1.625995
O	-1.612621	2.676617	1.280976
H	-2.473064	2.914658	1.630590
O	-2.295616	-1.941337	1.742571
H	-3.156801	-2.311706	1.941679
O	-3.028039	-2.102579	-0.789659
H	-3.293277	-1.657595	-1.596375
C	2.094953	-0.263217	-2.141324
H	2.927450	0.451553	-2.153584
C	2.068747	0.294753	1.467003
H	1.456541	0.345990	2.370265
C	2.526737	-1.069721	1.062121
H	3.557760	-1.167141	0.713905
H	2.245134	-1.899385	1.712304

C	3.018134	1.469616	1.321091
H	3.537590	1.464195	0.354033
H	2.489832	2.423212	1.404690
H	3.801399	1.443327	2.089954
H	2.517576	-1.262441	-2.320506
H	1.432937	-0.022620	-2.982319

E_{SCF}= -1324,064587 au
G_{423}= -1323,961262 au
E_{disp}= -35,9214 kcal·mol^{-1}

TS(44-38a)

Ta	0.791739	-0.248548	-0.008726
O	-0.789471	-1.356441	-0.191728
O	-0.355668	1.280761	0.176603
Si	-2.412624	-1.256108	-0.217303
Si	-1.944478	1.674880	0.254314
O	-2.832782	0.315919	0.038203
O	-3.142434	-2.095700	0.995916
H	-3.032114	-3.047867	0.997925
O	-2.910760	-1.778050	-1.696145
H	-3.842004	-1.690447	-1.906379
O	-2.404107	2.701367	-0.946069
H	-2.036818	3.586670	-0.933636
O	-2.173368	2.341276	1.740551
H	-3.075664	2.505547	2.019803
C	1.706545	-1.498883	-1.522427
H	2.774529	-1.316306	-1.680758
C	1.448857	-0.864884	1.901415
H	0.841276	-0.532828	2.742867
H	1.675053	-1.932543	1.960949
H	1.204750	-1.443823	-2.495019
C	2.554370	0.016324	1.444606
H	2.586762	0.972439	1.973680
H	2.377619	0.706554	0.077128
C	2.065430	1.433241	-1.150989
H	1.399936	1.284740	-2.010605
H	1.772770	2.387564	-0.703341
H	1.582686	-2.532807	-1.165462
C	3.508463	1.496752	-1.652237
H	4.210234	1.745853	-0.849949
H	3.832749	0.549944	-2.091682
H	3.617485	2.266105	-2.423804
C	3.933980	-0.609318	1.293001
H	4.645192	0.057128	0.798704
H	4.340331	-0.862721	2.278697
H	3.890528	-1.534475	0.710838

E_{SCF}= -1403,853402 au
G_{423}= -1403,682322 au
E_{disp}= -48,6745 kcal·mol^{-1}

TS(44-38b)

Ta	0.882464	-0.139961	-0.060395
O	-0.659047	-1.252268	-0.451892
O	-0.322452	1.297580	0.351608
Si	-2.283832	-1.203309	-0.495382
Si	-1.924303	1.618049	0.475617
O	-2.761710	0.287368	0.016275
O	-3.001604	-2.263058	0.540264
H	-2.898689	-3.197037	0.350942
O	-2.742395	-1.482672	-2.050969
H	-3.669535	-1.369303	-2.266994
O	-2.413342	2.820996	-0.533923
H	-2.073801	3.701650	-0.366673
O	-2.186866	2.006746	2.052313
H	-3.096142	2.094869	2.343161
C	1.863810	-1.066898	-1.756260
H	2.947150	-0.899290	-1.777115
C	1.533165	-1.053416	1.736615
H	0.872726	-0.805806	2.570941
H	1.459683	-0.761030	-2.727761
C	2.575041	-0.024471	1.464767
H	2.641976	0.803315	2.171537
H	2.413385	0.860442	0.263271
C	2.142389	1.751157	-0.856259
H	1.518320	1.749461	-1.757521
H	1.824571	2.617022	-0.267231
H	1.685080	-2.147743	-1.665222
C	3.610204	1.883200	-1.262099
H	4.276687	1.909229	-0.392742
H	3.932396	1.053769	-1.896894
H	3.780065	2.806968	-1.824779
C	1.927338	-2.522036	1.708875
H	2.539359	-2.764845	0.833762
H	2.516934	-2.787348	2.595441
H	1.046261	-3.168333	1.683566
H	3.565235	-0.407960	1.212579

E_{SCF}= -1403,854529 au
G_{423}= -1403,684735 au
E_{disp}= -48,3821 kcal·mol^{-1}

38b

Ta	0.844668	-0.285704	-0.234435
O	-0.653805	-1.420892	-0.244218
O	-0.217070	1.320663	0.123434
Si	-2.296720	-1.291723	-0.114509
Si	-1.788914	1.662576	0.385223
O	-2.650528	0.260981	0.250567
O	-2.877927	-2.202776	1.117898
H	-2.844353	-3.156447	1.025636
O	-2.895402	-1.752703	-1.570463
H	-3.817172	-1.570261	-1.760970
O	-2.439587	2.661733	-0.747305
H	-2.077182	3.546368	-0.818750
O	-1.908217	2.283955	1.901858
H	-2.785676	2.433651	2.258100
C	2.423135	-1.723011	-0.728184
H	3.440812	-1.320198	-0.795997
C	1.823618	0.036322	1.675148
H	1.004984	0.490597	2.253973
H	2.200120	-2.180749	-1.703507
C	2.931563	1.086036	1.538616
H	3.321780	1.366874	2.525963
H	2.579654	2.008037	1.065230
C	1.390409	0.674580	-2.099618

H	1.729598	-0.096015	-2.800742
H	0.452270	1.080414	-2.502835
H	2.446160	-2.541944	0.004464
C	2.433774	1.790652	-1.999263
H	2.100016	2.596589	-1.338711
H	3.391248	1.422203	-1.617656
H	2.633258	2.239618	-2.979530
C	2.302465	-1.200241	2.438755
H	3.183249	-1.647444	1.970513
H	2.577968	-0.930009	3.466964
H	1.533324	-1.976900	2.507978
H	3.778567	0.706353	0.956758

E_{SCF}= -1403,886059 au
G_{423}= -1403,714609 au
E_{disp}= -48,3063 kcal·mol^{-1}

45a

Ta	1.058967	0.265422	-0.411572
O	-0.370574	1.487629	-0.342132
O	-0.089002	-1.279935	-0.059348
Si	-1.996380	1.469173	-0.042806
Si	-1.683503	-1.545859	0.151137
O	-2.459312	-0.088807	0.122725
O	-2.848982	2.077043	-1.303904
H	-2.775354	3.015660	-1.484675
O	-2.203530	2.341429	1.330926
H	-3.051465	2.294447	1.775906
O	-2.049184	-2.184493	1.621612
H	-1.691781	-3.049520	1.829090
O	-2.188750	-2.504301	-1.084508
H	-3.130341	-2.661855	-1.173168
C	2.683616	1.673223	-0.799518
H	2.314420	2.223945	-1.686217
C	2.154025	-0.266266	1.363128
H	1.505310	-0.691706	2.134931
H	2.581415	2.395848	0.032061
H	2.868723	-1.048334	1.064749
C	4.156510	1.319064	-0.993647
H	4.559409	0.798286	-0.118278
H	4.295952	0.657243	-1.855058
H	4.786567	2.200535	-1.161694
C	1.534042	-0.656672	-2.300020
H	2.035549	0.062822	-2.959135
C	2.390092	-1.922396	-2.143577
H	1.878655	-2.629049	-1.480236
H	3.341673	-1.673420	-1.657011
H	2.727379	0.561441	1.789338
C	2.684031	-2.612126	-3.476826
H	3.293758	-3.510374	-3.335052
H	1.755254	-2.911059	-3.972430
H	3.223098	-1.944143	-4.156092
H	0.577245	-0.918327	-2.775241

E_{SCF}= -1403,889400 au
G_{423}= -1403,719082 au
E_{disp}= -46,517 kcal·mol^{-1}

45b

Ta	0.896910	-0.201609	-0.400324
O	-0.564947	-1.403404	-0.046561
O	-0.429926	1.201870	-0.402102
Si	-2.160221	-1.451663	0.300456
Si	-1.984701	1.517863	-0.006084
O	-2.734871	0.087172	0.283230
O	-2.482555	-2.019351	1.810184
H	-2.254898	-2.931663	1.996951
O	-2.856749	-2.384119	-0.860245
H	-3.813651	-2.441097	-0.871704
O	-2.813640	2.221110	-1.238172
H	-2.574482	3.117326	-1.479629
O	-1.959642	2.474168	1.333011
H	-2.788358	2.625617	1.791020
C	1.995995	-1.689539	0.763235
H	1.482566	-1.886533	1.712373
C	1.656548	-0.427332	-2.375669
H	0.889136	-0.267182	-3.141311
H	1.725418	-2.559073	0.131678
H	2.469756	0.289034	-2.555346
C	3.510766	-1.662478	0.965331
H	4.054126	-1.450958	0.037104
H	3.806299	-0.900171	1.692277
H	3.886390	-2.623049	1.338588
C	2.123211	1.239693	0.659237
H	3.128091	0.801882	0.530770
C	2.114454	2.589820	-0.073066
H	1.178134	3.122962	0.105874
H	2.233575	2.497534	-1.159811
C	1.853108	1.414318	2.151777
H	2.553543	2.129511	2.604131
H	0.843540	1.803545	2.320643
H	1.945936	0.472735	2.700731
H	2.940870	3.221670	0.279844
H	2.062660	-1.437895	-2.511568

E_{SCF}= -1403,887226 au
G_{423}= -1403,715826 au
E_{disp}= -48,4715 kcal·mol^{-1}

TS(45a-13)

Ta	0.594023	-0.747575	-0.115310
O	0.111108	1.097244	0.096790
O	-1.283007	-1.227779	-0.075840
Si	-1.223120	2.029875	0.290962
Si	-2.755452	-0.528252	-0.095813
O	-2.555973	1.088628	0.139582
O	-1.358072	3.179502	-0.876696
H	-0.704392	3.880468	-0.884339
O	-1.099974	2.697444	1.789056
H	-1.866879	3.156035	2.136494
O	-3.724159	-1.026476	1.136439
H	-3.951627	-1.957079	1.168293
O	-3.428786	-0.844456	-1.563246
H	-4.265831	-0.424707	-1.769132
C	2.672654	0.259199	-0.822518
H	2.129626	0.688646	-1.674891
H	3.446665	-0.378526	-1.265352

H	2.417238	-0.735684	0.245804
C	1.669804	-1.605950	1.259448
H	1.665193	-2.589683	0.728006
C	0.854327	-1.895572	-1.936231
H	0.337374	-2.857908	-1.822939
H	0.372750	-1.377632	-2.775087
H	1.894554	-2.094077	-2.210999
C	2.346484	-1.626957	2.594986
H	1.813446	-2.292022	3.283201
H	3.382354	-1.981828	2.537693
H	2.355412	-0.631410	3.045142
C	3.301938	1.385548	-0.000771
H	2.507267	1.978625	0.463047
H	3.883680	0.958037	0.826584
C	4.206411	2.298872	-0.826001
H	3.646420	2.781494	-1.633768
H	4.648678	3.087674	-0.208819
H	5.025567	1.736116	-1.285520

E_{SCF}= -1403,846048 au
G_{423}= -1403,677675 au
E_{disp}= -46,1080 kcal·mol^{-1}

TS(45b-13)

Ta	0.781360	-0.566691	-0.071995
O	-0.024057	1.168483	0.089451
O	-0.983398	-1.370588	-0.051822
Si	-1.500934	1.853792	0.278282
Si	-2.555569	-0.941185	-0.069296
O	-2.644912	0.689936	0.137043
O	-1.835493	2.953358	-0.897616
H	-1.346371	3.777555	-0.883655
O	-1.497113	2.547840	1.769791
H	-2.336252	2.848607	2.122748
O	-3.414414	-1.577870	1.181059
H	-3.471894	-2.533222	1.233769
O	-3.173447	-1.397494	-1.524189
H	-4.073835	-1.137168	-1.726156
C	2.747341	0.817967	-0.714885
H	3.686501	0.290802	-0.936702
H	2.554041	-0.209953	0.311438
C	1.944123	-1.172155	1.361633
H	2.136612	-2.160682	0.878962
C	1.317799	-1.766505	-1.796398
H	1.062318	-2.809695	-1.560417
H	0.723288	-1.491851	-2.675025
H	2.377489	-1.731723	-2.068479
C	2.562645	-1.015411	2.715761
H	2.140415	-1.746373	3.414176
H	3.648171	-1.169736	2.703044
H	2.366309	-0.021689	3.124958
C	3.054326	1.973701	0.241757
H	2.139381	2.507561	0.512756
H	3.526213	1.632631	1.169150
C	2.229758	1.361332	-2.055742
H	2.961063	2.068725	-2.471921
H	2.081248	0.576966	-2.800548
H	1.288352	1.903549	-1.934128
H	3.735465	2.694731	-0.226613

E_{SCF}= -1403,838375 au
G_{423}= -1403,668214 au
E_{disp}= -48,5561 kcal·mol^{-1}

TS(15-19)

Ta	-1.087438	-0.364207	-0.078761
O	-0.005287	1.218807	0.198165
O	0.529288	-1.368187	-0.328609
Si	1.546528	1.692870	0.319299
Si	2.156699	-1.192320	-0.262842
O	2.500317	0.376211	0.062974
O	1.955963	2.232932	1.819588
H	1.515455	3.022834	2.137142
O	1.789062	2.851089	-0.823359
H	2.681163	3.182709	-0.938160
O	2.891189	-1.517820	-1.697975
H	2.859724	-2.421834	-2.015084
O	2.675487	-2.203558	0.925927
H	3.593224	-2.138818	1.195591
C	-2.462163	0.848074	-1.251732
H	-3.385565	0.253645	-1.346224
C	-1.835176	-0.605753	1.882253
H	-1.115582	-0.881269	2.651914
H	-2.475256	0.218419	2.203143
H	-2.091381	0.968133	-2.278320
C	-2.486813	-1.702355	1.120726
H	-2.180696	-2.715911	1.380961
H	-3.568018	-1.637880	0.994443
H	-2.179291	-1.851890	-0.365764
C	-2.786728	2.221918	-0.648711
H	-1.899205	2.857839	-0.630306
H	-3.563557	2.738677	-1.225116
H	-3.155046	2.150625	0.381048
C	-1.796415	-1.949949	-1.731845
H	-2.827657	-2.042937	-2.083597
H	-1.245534	-1.399677	-2.500757
H	-1.346769	-2.943257	-1.660105

E_{SCF}= -1364,544320 au
G_{423}= -1364,398686 au
E_{disp}= -43,9613 kcal·mol^{-1}

X. Comparison between 2T and 9T clusters

X1. Cluster 2T

Hydrogen molecule

H	0.671701	0.570934	0.000000
H	-0.071701	0.570934	0.000000

E_{SCF}= -1,177517 au

Ethane

C	-1.795977	1.777601	0.005902
H	-1.449146	0.739316	-0.026078
H	-1.448247	2.268420	-0.909265
H	-2.890493	1.759462	-0.026617
C	-1.287454	2.496742	1.251503
H	-1.633551	3.535286	1.283034
H	-1.635918	2.006443	2.166669
H	-0.192940	2.514103	1.284471

E_{SCF}= -79,808444 au

Ethene

C	-1.385929	1.505198	-0.000005
C	-0.056321	1.505183	0.000002
H	-1.959334	2.428460	0.000008
H	-1.959354	0.581948	-0.000026
H	0.517084	0.581920	-0.000013
H	0.517104	2.428433	0.000020

E_{SCF}= -78,560013 au

1a (singlet)

Ta	1.504323	-0.010653	-0.005918
O	0.435607	-1.519844	0.071006
O	0.462627	1.517511	-0.078496
Si	-1.238239	-1.529414	0.058243
Si	-1.210766	1.557136	-0.058654
O	-1.787309	0.018833	-0.001270
O	-1.831078	-2.155991	1.449853
H	-1.586424	-3.066004	1.642146
O	-1.656496	-2.381205	-1.275498
H	-2.543385	-2.229899	-1.614937
O	-1.797856	2.198081	-1.446098
H	-1.537639	3.104033	-1.637080
O	-1.608175	2.412661	1.279079
H	-2.495859	2.275554	1.622442
H	3.289281	-0.026738	-0.008939

E_{SCF}= -1166,527358 au

TS(1a-1b)

Ta	1.31025	-0.20773	0.02935
O	0.75582	1.57595	-0.21605
O	0.21795	-1.73676	-0.12439
Si	-0.89686	1.72909	-0.01237
Si	-1.40510	-1.36293	-0.00585
O	-1.59524	0.25475	-0.29336
O	-1.54156	2.68859	-1.17561
H	-1.18389	3.57991	-1.22646
O	-1.13695	2.28889	1.50817
H	-2.03004	2.21034	1.85610
O	-2.02015	-1.64676	1.48819
H	-1.91994	-2.54287	1.82339
O	-2.13542	-2.22765	-1.19107
H	-3.04285	-1.98238	-1.39427
H	0.59661	-0.15993	-2.19346
H	1.36260	-0.27939	-2.10036
H	2.44107	-0.36340	1.38018

E_{SCF}= -1167,687725 au

1b

Ta	1.434010	-0.008428	-0.002875
O	0.388826	-1.558520	0.071644
O	0.416570	1.560151	-0.074182
Si	-1.282032	-1.545017	0.048335
Si	-1.254234	1.576324	-0.047463
O	-1.785550	0.020216	-0.000616
O	-1.902812	-2.161215	1.431853
H	-1.660696	-3.068812	1.639240
O	-1.703861	-2.366130	-1.302137
H	-2.613913	-2.269360	-1.597633
O	-1.866680	2.206026	-1.428586
H	-1.607269	3.108849	-1.635888
O	-1.658445	2.402126	1.305518
H	-2.569605	2.321682	1.602478
H	3.180941	-0.023820	-0.005712
H	2.164753	0.050243	1.584160
H	2.158430	-0.080553	-1.592252

E_{SCF}= -1167,774135 au

TS(1a-3a)

Ta	1.014895	-0.011506	-0.346183
O	-0.029086	1.537143	-0.149506
O	-0.042386	-1.541908	-0.101730
Si	-1.661337	1.552138	0.161296
Si	-1.683741	-1.541521	0.168342
O	-2.210157	0.009329	0.319036
O	-2.511574	2.192240	-1.088272
H	-2.223801	3.060347	-1.385864
O	-1.835529	2.392487	1.560007
H	-2.701641	2.335783	1.974153
O	-2.049268	-2.265694	1.595241
H	-1.880735	-3.211589	1.634863
O	-2.366021	-2.295481	-1.119034
H	-3.275696	-2.048251	-1.309040
C	3.161980	0.004022	0.882422
H	2.926496	0.897079	1.467755
H	2.928989	-0.865028	1.503541
C	4.658256	-0.001578	0.505303
H	5.278574	0.018815	1.407126
H	4.921594	-0.897222	-0.067243
H	4.918617	0.869849	-0.104761
H	1.933623	-0.033647	-1.848830
H	2.832105	-0.020124	-0.330759

E_{SCF}= -1246,322015 au

TS(1b-2)

Ta	1.066277	0.372319	-0.407398
O	0.209200	-1.330175	-0.301354

O	-0.419038	1.476832	-0.025414
Si	-1.357088	-1.781284	-0.032968
Si	-2.000695	1.164755	0.347538
O	-2.280557	-0.451121	0.260189
O	-1.485950	-2.704617	1.320624
H	-1.085280	-3.576905	1.262876
O	-1.856856	-2.563967	-1.386910
H	-2.805236	-2.547160	-1.545438
O	-3.019920	1.849110	-0.741044
H	-2.935158	2.800857	-0.850222
O	-2.208703	1.725489	1.877398
H	-3.015917	1.441227	2.316512
C	2.802966	-0.697665	0.726201
C	4.232096	-0.273000	1.062225
H	4.684704	0.260185	0.221011
H	4.261978	0.394786	1.931532
H	4.860646	-1.138958	1.297303
H	0.983262	0.450296	-2.140299
H	2.553518	1.000750	-1.147839
H	1.904994	1.570723	0.805706
H	2.822134	-1.368569	-0.150065
H	2.349249	-1.261870	1.550699
H	2.354391	0.730916	0.873404

E_{SCF}= -1247,537588 au

2

Ta	0.786724	-0.191003	-0.695903
O	-0.420805	-1.496240	-0.113050
O	-0.152975	1.432489	-0.304002
Si	-1.985056	-1.385112	0.451684
Si	-1.664733	1.651561	0.316718
O	-2.355366	0.195573	0.671515
O	-2.120900	-2.085619	1.927740
H	-2.006745	-3.040256	1.950388
O	-2.919296	-2.094800	-0.693502
H	-3.845682	-1.836355	-0.699502
O	-2.679230	2.342273	-0.775172
H	-2.350342	3.145153	-1.190437
O	-1.462333	2.542592	1.680519
H	-2.233425	2.611076	2.251151
C	2.411032	-0.134808	0.714115
H	1.971718	0.355957	1.601447
H	2.382343	-1.219497	0.945481
C	3.860390	0.298540	0.523761
H	4.298316	-0.184985	-0.354627
H	3.934686	1.382612	0.379746
H	0.529981	0.092559	-2.409703
H	2.068826	-0.982485	-1.658040
H	1.862103	1.252075	-1.889300
H	2.298436	1.277053	-1.257037
H	4.483527	0.047681	1.391323

E_{SCF}= -1247,563230 au

3a

Ta	0.933820	0.436051	-0.204620
O	-0.187463	1.909781	0.097277
O	-0.040015	-1.172355	-0.346722
Si	-1.834155	1.798259	0.345814
Si	-1.686626	-1.274401	-0.141500
O	-2.281872	0.225630	0.190112
O	-2.659518	2.608363	-0.815527
H	-2.518251	3.559244	-0.847606
O	-2.095329	2.364898	1.859395
H	-2.929470	2.117462	2.269131
O	-2.082127	-2.189352	1.159119
H	-1.688297	-3.066400	1.190572
O	-2.266430	-1.848897	-1.562263
H	-3.221835	-1.829202	-1.670332
C	1.639825	0.608383	-2.234802
H	0.711663	0.507169	-2.831499
H	1.965658	1.653025	-2.362904
C	2.711280	-0.337968	-2.776150
H	2.893919	-0.181446	-3.847065
H	3.658715	-0.192443	-2.248367
H	2.422761	-1.388085	-2.651040
H	1.621762	0.040447	1.362185
H	2.667218	0.670543	-0.139965

E_{SCF}= -1246,386730 au

3b

Ta	-0.716857	0.857007	0.106039
O	0.930117	1.732216	0.216875
O	-0.137367	-0.971217	0.125672
Si	2.509437	1.200725	0.191207
Si	1.374135	-1.627001	0.130881
O	2.511237	-0.436036	0.249330
O	3.315125	1.700743	1.528427
H	3.472124	2.647329	1.592957
O	3.147599	1.779179	-1.204241
H	3.912081	1.304230	-1.543439
O	1.716938	-2.395520	-1.280360
H	1.048102	-3.018460	-1.580213
O	1.430755	-2.611071	1.443924
H	2.302310	-2.944306	1.676714
C	-2.023853	0.673338	1.776667
H	-1.631133	0.055206	2.588553
H	-2.399033	1.620044	2.170044
C	-3.017713	-0.047929	0.878143
H	-3.160532	-1.094546	1.155015
H	-3.977337	0.465283	0.801286
H	-2.684396	-0.097057	-0.206342
H	-1.248941	0.546670	-1.528453
H	-1.900676	2.131947	-0.353604

E_{SCF}= -1246,387813 au

TS(3b-4)

Ta	-1.171209	-0.381810	-0.379771
O	-0.193055	1.260452	-0.218012
O	0.248352	-1.574146	-0.065503
Si	1.370332	1.652127	0.107488
Si	1.866456	-1.360937	0.210749
O	2.224278	0.240601	0.242167
O	1.362479	2.506276	1.505330
H	2.132735	3.062152	1.651990
O	2.077529	2.581198	-1.046391

H	2.456380	2.104136	-1.790588
O	2.762646	-1.982075	-1.018215
H	2.575020	-2.898683	-1.241752
O	2.160864	-2.077872	1.658254
H	3.038949	-1.935834	2.023612
C	-2.828981	1.232680	0.676726
H	-2.161775	1.955659	1.132229
H	-3.325446	1.521827	-0.247514
C	-3.209411	0.105923	1.341598
H	-2.851758	-0.097295	2.347703
H	-4.015526	-0.523998	0.984330
H	-2.102568	-1.388006	0.767341
H	-1.014341	-0.566797	-2.102823
H	-2.719158	-0.780449	-1.151029

E_{SCF}= -1246,333533 au

4

Ta	-1.079938	-0.564453	0.143229
O	-0.273847	1.150460	0.395704
O	0.405253	-1.684657	0.008424
Si	1.308194	1.613948	0.496740
Si	2.037539	-1.344832	0.039345
O	2.244360	0.266780	0.253978
O	1.520069	2.255972	1.984234
H	2.246235	2.879600	2.069325
O	1.732858	2.731027	-0.627903
H	2.092724	2.380651	-1.448036
O	2.732703	-1.683981	-1.407319
H	2.666688	-2.597710	-1.700945
O	2.634913	-2.227150	1.283454
H	3.524119	-2.005843	1.574821
C	-3.198435	1.175549	-0.360502
H	-2.591458	1.971905	-0.781101
H	-3.825231	0.616146	-1.046014
C	-3.256536	0.969065	0.971581
H	-2.697791	1.592105	1.664216
H	-3.932119	0.237392	1.400338
H	-1.842608	-0.837537	1.700469
H	-1.683825	-0.338854	-1.488367
H	-2.570835	-1.514627	-0.086491

E_{SCF}= -1246,344110 au

TS(3a-5)

Ta	1.17488	-0.16741	-0.29255
O	-0.19068	-1.43783	0.03673
O	0.06060	1.37260	-0.07158
Si	-1.83720	-1.37320	0.18988
Si	-1.55462	1.63479	0.07469
O	-2.32250	0.19148	0.28429
O	-2.32925	-2.07918	1.58869
H	-2.18650	-3.02846	1.64363
O	-2.44622	-2.11516	-1.14492
H	-3.35746	-1.89219	-1.35752
O	-2.21751	2.27690	-1.28759
H	-1.81632	3.09696	-1.59031
O	-1.74732	2.59871	1.39140
H	-2.64916	2.67631	1.71600
C	2.74636	-0.37400	0.88437
H	2.89689	-1.13536	1.65558
H	2.66119	-1.29374	-0.47201
C	3.83600	0.68005	0.82533
H	4.81090	0.24526	0.57265
H	3.63594	1.46074	0.08007
H	3.93109	1.17001	1.80165
H	1.81727	0.52079	-1.80101
H	2.02446	-1.55771	-1.23118

E_{SCF}= -1246,345365 au

5

Ta	1.16079	-0.27862	-0.30255
O	-0.25248	-1.50910	0.02824
O	0.20993	1.36061	-0.21104
Si	-1.87900	-1.28408	0.23196
Si	-1.38649	1.71333	0.00717
O	-2.23257	0.31952	0.23114
O	-2.38602	-1.84707	1.68916
H	-2.27955	-2.79286	1.82611
O	-2.59262	-2.05154	-1.03481
H	-3.50004	-1.78851	-1.21552
O	-2.04913	2.41121	-1.32516
H	-1.64690	3.24064	-1.59944
O	-1.46424	2.67199	1.33838
H	-2.33471	2.74945	1.73983
C	2.59779	-0.32258	0.99275
H	2.77837	-0.98312	1.84468
H	2.38212	-1.92183	-0.69289
C	3.50961	0.88799	0.91529
H	4.55294	0.59220	0.74849
H	3.25146	1.56320	0.08572
H	3.46680	1.47747	1.84056
H	2.00875	0.05568	-1.83423
H	1.79284	-2.09982	-1.18047

E_{SCF}= -1246,351381 au

6

Ta	1.183465	0.054474	-0.561247
O	0.139298	-1.515635	-0.508348
O	0.168057	1.634619	-0.273693
Si	-1.470485	-1.507908	-0.083478
Si	-1.403824	1.587833	0.255028
O	-1.880294	0.015534	0.381747
O	-1.760470	-2.445977	1.228481
H	-1.538622	-3.377217	1.136393
O	-2.281283	-1.982935	-1.427555
H	-3.228203	-1.814026	-1.428317
O	-2.425893	2.265389	-0.837098
H	-2.220453	3.170214	-1.091195
O	-1.420064	2.328469	1.716755
H	-2.226654	2.231738	2.231373
C	2.425541	0.233103	-1.999523
C	3.159829	-0.426711	-3.127397
H	2.571477	1.336634	-1.946660
H	4.244277	-0.289933	-3.025509
H	2.967012	-1.503751	-3.155492

H	2.380818	-0.025892	0.723188
H	2.872721	-0.013608	-4.103356

E_{SCF}= -1245,179785 au

X2. Cluster 9T

Hydrogen molecule

H	0.671701	0.570934	0.000000
H	-0.071701	0.570934	0.000000

E_{SCF}= -1,177517 au

Ethane

C	-1.795977	1.777601	0.005902
H	-1.449146	0.739316	-0.026078
H	-1.448247	2.268420	-0.909265
H	-2.890493	1.759462	-0.026617
C	-1.287454	2.496742	1.251503
H	-1.633551	3.535286	1.283034
H	-1.635918	2.006443	2.166669
H	-0.192940	2.514103	1.284471

E_{SCF}= -79,808444 au

Ethene

C	-1.385929	1.505198	-0.000005
C	-0.056321	1.505183	0.000002
H	-1.959334	2.428460	0.000008
H	-1.959354	0.581948	-0.000026
H	0.517084	0.581920	-0.000013
H	0.517104	2.428433	0.000020

E_{SCF}= -78,560013 au

1a (singlet)

Ta	-4.221545	-0.246152	0.107918
O	-3.343100	1.399019	0.111338
O	-3.109730	-1.735352	-0.041018
Si	-1.690756	1.523967	0.009034
Si	-1.456067	-1.606346	-0.098576
O	-1.107109	-0.003957	-0.143808
O	-1.036863	2.202730	1.347199
O	-1.214702	2.386390	-1.299370
O	-0.820696	-2.308293	-1.434978
O	-0.753545	-2.269377	1.223649
H	-5.982041	-0.385588	0.260784
Si	0.570072	2.616126	1.442421
Si	0.383506	2.758077	-1.569913
Si	0.819047	-2.438836	-1.678925
Si	0.881080	-2.533144	1.349311
O	1.478630	-2.617777	-0.176516
O	1.046053	3.009709	-0.079441
O	1.543268	-1.309503	2.188175
O	1.391043	1.336244	2.008349
O	1.113803	1.526313	-2.335007
O	1.392199	-1.103718	-2.402690
Si	2.334407	0.094966	2.458661
Si	2.205615	0.309979	-2.279120
O	0.521968	4.064585	-2.533050
H	0.133182	4.882795	-2.211736
O	1.179994	-3.964054	2.077528
H	0.991493	-4.014843	3.018726
O	1.156878	-3.686072	-2.670422
H	0.872906	-4.558800	-2.385197
O	0.779763	3.922273	2.395117
H	0.919047	3.750446	3.330534
O	3.294962	0.449867	-3.490659
H	2.984927	0.250462	-4.378377
O	3.010622	0.401787	-0.873343
O	3.760031	0.082267	1.657565
O	2.632727	0.265710	4.060123
H	3.506638	-0.014471	4.345339
Si	4.292720	0.186464	0.108292
O	5.019154	-1.205436	-0.369039
H	5.788307	-1.483497	0.135534
O	5.305262	1.477770	0.098019
H	5.601489	1.764009	-0.771150

E_{SCF}= -4399,537565 au

TS(1a-1b)

Ta	-4.06156	-0.28091	0.01548
O	-3.45112	1.50777	0.21908
O	-3.13343	-1.94370	0.10813
Si	-1.80257	1.55555	0.11737
Si	-1.50929	-1.67100	0.00959
O	-1.34407	-0.03727	0.17867
O	-1.11027	2.29553	1.40403
O	-1.24930	2.25484	-1.25204
O	-0.83709	-2.17273	-1.39786
O	-0.68141	-2.37694	1.23676
H	-5.40583	-0.36643	-1.12346
Si	0.51348	2.63846	1.48048
Si	0.30639	2.77156	-1.52691
Si	0.77935	-2.32099	-1.71582
Si	0.96165	-2.54134	1.31656
O	1.52804	-2.51222	-0.23945
O	0.97113	3.04241	-0.04331
O	1.59259	-1.32388	2.18319
O	1.27149	1.29655	1.99440
O	1.11833	1.62507	-2.34002
O	1.37073	-0.99997	-2.43637
Si	2.31411	0.13132	2.43225
Si	2.20760	0.40908	-2.31469
O	0.32610	4.10262	-2.46474
H	-0.07467	4.89833	-2.10444
O	1.37928	-3.98649	1.94562
H	1.37552	-4.06528	2.90349
O	1.06253	-3.57503	-2.71417
H	0.63553	-4.41129	-2.50901
O	0.79982	3.91043	2.45654
H	0.95479	3.71536	3.38492
O	3.26616	0.54206	-3.55130
H	2.89873	0.58642	-4.43853
O	3.03256	0.45049	-0.92108
O	3.70949	0.18351	1.59155
O	2.63328	0.33406	4.02432
H	3.51962	0.08019	4.29746

Si	4.20033	-0.16580	0.05969
O	4.37534	-1.77018	-0.21294
H	3.55105	-2.26785	-0.31383
O	5.64543	0.57088	-0.11058
H	6.17195	0.28846	-0.86338
H	-3.85333	-0.33081	2.15794
H	-3.07937	-0.25890	2.19196

E_{SCF}= -4400,704765 au

1b

Ta	-4.182673	-0.247658	0.107108
O	-3.371482	1.457043	0.135308
O	-3.092413	-1.786295	0.033988
Si	-1.723267	1.565199	0.016882
Si	-1.447925	-1.606583	-0.060716
O	-1.199608	0.014443	-0.156240
O	-1.037969	2.206840	1.357019
O	-1.232025	2.416596	-1.291390
O	-0.805674	-2.306489	-1.392650
O	-0.694581	-2.192656	1.268481
H	-4.971728	-0.268498	-1.446204
Si	0.581526	2.576332	1.438529
Si	0.369826	2.776060	-1.564584
Si	0.831846	-2.423986	-1.661418
Si	0.928525	-2.533575	1.367088
O	1.511414	-2.576778	-0.165341
O	1.036065	3.022762	-0.075037
O	1.655080	-1.380828	2.255455
O	1.363152	1.235046	1.913979
O	1.083368	1.534276	-2.327992
O	1.379102	-1.089151	-2.403552
Si	2.378327	0.078602	2.428925
Si	2.189319	0.329088	-2.305286
O	0.516692	4.080447	-2.528005
H	0.129605	4.901550	-2.211941
O	1.171446	-4.004638	2.032419
H	0.979059	-4.093522	2.969979
O	1.165748	-3.677559	-2.644614
H	0.893785	-4.551068	-2.350128
O	0.850080	3.827551	2.445962
H	1.010418	3.610164	3.368599
O	3.240649	0.479168	-3.547564
H	2.895330	0.329836	-4.432118
O	3.033171	0.422926	-0.924049
O	3.788664	0.080879	1.604509
O	2.673821	0.370690	4.012610
H	3.504060	0.028332	4.354836
Si	4.316854	0.209631	0.055535
O	5.057696	-1.167857	-0.439627
H	5.827866	-1.446650	0.063050
O	5.312420	1.513674	0.060523
H	5.608578	1.812691	-0.804331
H	-5.909191	-0.399419	0.156612
H	-4.874287	-0.357593	1.702461

E_{SCF}= -4400,784556 au

TS(1a-3a)

Ta	3.946370	0.003411	-0.252598
O	2.961937	-1.613438	-0.260298
O	2.925212	1.588661	-0.103762
Si	1.314622	-1.602268	-0.216307
Si	1.276995	1.551171	-0.145424
O	0.837980	-0.028698	-0.252271
O	0.739067	-2.284680	1.162623
O	0.617920	-2.368474	-1.489070
O	0.662454	2.351257	-1.438336
O	0.604991	2.184492	1.211708
Si	-0.881948	-2.518746	1.418253
Si	-1.022714	-2.602927	-1.601152
Si	-0.961903	2.608114	-1.655270
Si	-0.986085	2.628255	1.364792
O	-1.584366	2.852643	-0.145667
O	-1.564754	-2.780533	-0.051655
O	-1.791163	1.464964	2.166668
O	-1.472370	-1.177558	2.121783
O	-1.733478	-1.329521	-2.315404
O	-1.645602	1.315105	-2.359671
Si	-2.468534	0.031053	2.554314
Si	-2.638972	0.025802	-2.198065
O	-1.357348	-3.898554	-2.531707
H	-0.976098	-4.737287	-2.258312
O	-1.118114	4.050913	2.157765
H	-0.987986	4.025110	3.109442
O	-1.223209	3.877175	-2.644110
H	-0.842510	4.717940	-2.375905
O	-1.147806	-3.836881	2.343568
H	-1.120564	-3.698766	3.294453
O	-3.797556	0.037593	-3.352512
H	-3.524510	-0.214907	-4.238871
O	-3.371599	0.121846	-0.753896
O	-3.932758	-0.104287	1.840078
O	-2.659517	-0.086588	4.177879
H	-3.427478	0.368286	4.534805
Si	-4.571307	-0.076116	0.328462
O	-5.613111	1.192612	0.334194
H	-5.982941	1.425942	-0.522461
O	-5.295280	-1.504358	-0.030998
H	-5.972040	-1.804931	0.581636
C	5.931969	-0.050739	1.272210
H	5.595175	0.800838	1.868272
H	5.610489	-0.962334	1.781719
C	7.465660	-0.030188	1.117851
H	7.803373	0.882337	0.616145
H	7.944975	-0.074194	2.100763
H	7.818094	-0.883792	0.529967
H	5.754509	0.008124	0.061747
H	5.088627	0.081278	-1.582504

E_{SCF}= -4479,334460 au

TS(1b-2)

Ta	4.068359	0.247839	-0.439142
O	2.751568	1.615554	-0.348657
O	2.951560	-1.311601	-0.257295
Si	1.127175	1.590355	-0.102427

Si	1.328425	-1.469874	-0.128693
O	0.663712	0.024187	0.051162
O	0.295345	2.259229	-1.348273
O	0.705197	2.371645	1.279629
O	0.861460	-2.347440	1.183350
O	0.664946	-2.163977	-1.462695
H	5.686808	0.581384	-1.071189
H	5.271579	0.563928	0.927147
Si	-1.321809	2.627847	-1.272534
Si	-0.883531	2.573399	1.719640
Si	-0.745578	-2.643502	1.477185
Si	-0.960158	-2.481461	-1.539824
O	-1.466379	-2.771064	-0.002703
O	-1.712385	2.807584	0.310843
O	-1.696963	-1.181906	-2.181979
O	-2.177281	1.435147	-1.970771
O	-1.413340	1.252444	2.504347
O	-1.402873	-1.436847	2.346236
Si	-2.815905	-0.015611	-2.361164
Si	-2.332614	-0.091788	2.402785
O	-1.054282	3.828862	2.744440
H	-0.819798	4.696396	2.403588
O	-1.257057	-3.822245	-2.423082
H	-1.298950	-3.701242	-3.375854
O	-0.937282	-3.993806	2.372912
H	-0.636624	-4.816626	1.977427
O	-1.625303	4.054025	-2.009870
H	-1.562098	4.063889	-2.968761
O	-3.280263	-0.160553	3.734263
H	-3.352243	-1.028408	4.141249
O	-3.212495	0.032448	1.036753
O	-4.136754	-0.305687	-1.439678
O	-3.250939	-0.042653	-3.940217
H	-4.075607	0.405404	-4.147943
Si	-4.551168	-0.214322	0.144715
O	-5.599387	1.046297	0.238649
H	-5.828292	1.331378	1.128111
O	-5.201661	-1.630649	0.665180
H	-5.940496	-1.972368	0.154016
C	5.496725	-0.927272	0.959648
H	5.508810	-1.669907	0.141887
H	4.876817	-1.345654	1.762052
C	6.928899	-0.678823	1.431327
H	7.389324	-1.602157	1.798762
H	7.544968	-0.290290	0.615131
H	6.964370	0.049144	2.250377
H	4.180964	0.113934	-2.164175
H	4.965635	1.442934	0.723791

E_{SCF}= -4480,549151 au

2

Ta	4.052212	-0.202579	-0.437161
O	2.963965	1.389326	-0.356088
O	2.826357	-1.595002	-0.111106
Si	1.341058	1.513758	-0.188721
Si	1.179974	-1.564959	0.026708
O	0.718746	0.004951	0.045595
O	0.602501	2.146792	-1.511821
O	0.913223	2.415612	1.117990
O	0.667526	-2.263679	1.420110
O	0.450647	-2.318738	-1.233787
H	5.550997	-0.937872	-1.054849
H	5.280722	1.262737	-1.407133
Si	-1.021758	2.483684	-1.531020
Si	-0.679532	2.737320	1.459415
Si	-0.949811	-2.445703	1.762728
Si	-1.176652	-2.650783	-1.254748
O	-1.688364	-2.678458	0.304782
O	-1.436909	2.904381	0.002738
O	-1.938766	-1.504875	-2.119402
O	-1.817165	1.152743	-2.014139
O	-1.322086	1.515555	2.317740
O	-1.525946	-1.118175	2.499118
Si	-2.763429	-0.114047	-2.372037
Si	-2.381226	0.270151	2.357729
O	-0.818944	4.078050	2.377582
H	-0.495198	4.896405	1.990986
O	-1.453504	-4.130204	-1.890741
H	-1.307004	-4.224360	-2.836048
O	-1.186237	-3.686455	2.792300
H	-0.938487	-4.561114	2.480414
O	-1.345960	3.747098	-2.510708
H	-1.549855	3.532383	-3.425180
O	-3.417165	0.435756	3.613215
H	-3.041929	0.373768	4.495953
O	-3.255798	0.273540	0.992043
O	-4.136440	-0.132690	-1.483854
O	-3.156947	0.017519	-3.956839
H	-3.997168	-0.375711	-4.207569
Si	-4.587353	0.038144	0.084547
O	-5.585457	1.341253	0.100238
H	-5.818827	1.671064	0.973100
O	-5.304769	-1.326244	0.648306
H	-6.111876	-1.598737	0.203479
C	5.299966	-0.003488	1.294346
H	5.265365	-1.082712	1.553150
H	4.635137	0.484552	2.030861
C	6.729496	0.504588	1.437422
H	7.135519	0.312961	2.438166
H	7.388035	0.020979	0.709868
H	6.783948	1.586420	1.270969
H	4.184649	0.015321	-2.169274
H	5.569876	1.315202	-0.695384

E_{SCF}= -4480,573702 au

3a

Ta	3.904827	-0.461511	-0.457117
O	3.146557	1.280050	-0.452658
O	2.752806	-1.952855	-0.253401
Si	1.519424	1.448691	-0.236492
Si	1.124175	-1.703153	-0.119234
O	0.934159	-0.076134	-0.020577
O	0.761069	2.116348	-1.525838
O	1.149368	2.322375	1.099524

O	0.483685	-2.373526	1.231804
O	0.310897	-2.270448	-1.423709
H	5.574855	-0.780504	-0.794419
Si	-0.847343	2.529409	-1.487234
Si	-0.405340	2.779012	1.474523
Si	-1.149829	-2.394676	1.543360
Si	-1.322541	-2.554855	-1.476654
O	-1.877025	-2.546552	0.068343
O	-1.152664	3.072865	0.032350
O	-2.037411	-1.390313	-2.366982
O	-1.709262	1.184566	-1.794386
O	-1.136841	1.581599	2.289291
O	-1.602953	-1.017781	2.261437
Si	-2.775018	0.074472	-2.305136
Si	-2.313126	0.449835	2.383157
O	-0.409634	4.092166	2.438476
H	-0.028929	4.896572	2.075322
O	-1.635494	-4.028038	-2.108638
H	-1.424044	-4.155168	-3.037751
O	-1.524899	-3.610763	2.560166
H	-1.321249	-4.502810	2.265946
O	-1.177821	3.717214	-2.550786
H	-1.526761	3.440751	-3.403090
O	-3.124966	0.567614	3.795841
H	-2.662313	0.272820	4.584971
O	-3.368505	0.712849	1.177224
O	-4.065808	-0.038422	-1.314521
O	-3.244999	0.523590	-3.808431
H	-4.082566	0.168061	-4.117763
Si	-4.594599	0.241368	0.212462
O	-5.699085	1.443889	0.055304
H	-6.023734	1.817405	0.879903
O	-5.203368	-1.133588	0.869156
H	-5.774612	-1.663610	0.307001
C	4.995826	-0.381833	1.396123
H	5.295688	-1.414912	1.631513
H	4.197917	-0.127425	2.123808
C	6.184660	0.560833	1.577924
H	6.554097	0.557254	2.611246
H	7.012295	0.270209	0.923836
H	5.919937	1.595784	1.333914
H	4.288653	-0.493434	-2.166676

E_{SCF}= -4479,397675 au

3b

Ta	4.11354	-0.32991	-0.25735
O	3.02852	1.26764	-0.23245
O	2.82234	-1.66989	0.01789
Si	1.40760	1.44862	-0.12026
Si	1.17299	-1.61592	0.09954
O	0.73296	-0.04022	0.09715
O	0.72721	2.10013	-1.46549
O	0.96776	2.36698	1.17133
O	0.60029	-2.30290	1.47558
O	0.47603	-2.36215	-1.18409
H	5.55673	-1.22361	-0.82837
Si	-0.88369	2.48980	-1.53302
Si	-0.62506	2.73089	1.46673
Si	-1.03206	-2.44407	1.76005
Si	-1.15945	-2.64114	-1.26401
O	-1.72441	-2.66117	0.27744
O	-1.33463	2.91788	-0.01159
O	-1.85282	-1.46464	-2.14466
O	-1.70780	1.18968	-2.05063
O	-1.32363	1.52700	2.30642
O	-1.60332	-1.10264	2.47492
Si	-2.65757	-0.06904	-2.42860
Si	-2.41484	0.30945	2.31170
O	-0.75590	4.07637	2.37937
H	-0.41454	4.88811	1.99403
O	-1.46206	-4.10665	-1.91983
H	-1.30617	-4.19307	-2.86439
O	-1.33483	-3.67632	2.78281
H	-1.07964	-4.55503	2.48877
O	-1.13634	3.76946	-2.51326
H	-1.29027	3.56890	-3.44061
O	-3.48139	0.49105	3.53902
H	-3.15935	0.29767	4.42370
O	-3.24706	0.35065	0.91955
O	-4.05627	-0.06534	-1.58050
O	-3.01092	0.04899	-4.02407
H	-3.88781	-0.25655	-4.27151
Si	-4.55151	0.11476	-0.02643
O	-5.54427	1.42190	-0.04738
H	-5.80122	1.75805	0.81639
O	-5.29082	-1.24406	0.52266
H	-6.07990	-1.52185	0.04968
C	5.46091	0.31424	1.25334
H	6.12887	-0.46512	1.62597
H	4.98614	0.83651	2.08847
C	6.10538	1.23500	0.22973
H	7.15910	1.01327	0.05585
H	5.66301	1.12310	-0.81169
H	5.96310	2.29322	0.45748
H	4.37689	0.04360	-1.93666

E_{SCF}= -4479,398126 au

TS(3b-4)

Ta	4.121386	0.176042	-0.393138
O	2.816172	1.538814	-0.375845
O	2.993413	-1.375345	-0.095313
Si	1.186992	1.540975	-0.146887
Si	1.370045	-1.514191	-0.011566
O	0.705389	-0.010710	0.074656
O	0.378674	2.156380	-1.435045
O	0.757948	2.394915	1.188662
O	0.862047	-2.319968	1.333244
O	0.728338	-2.275928	-1.320648
H	5.748487	0.387547	-1.043761
Si	-1.234763	2.545056	-1.397734
Si	-0.833034	2.638230	1.597542
Si	-0.753662	-2.583731	1.605311
Si	-0.898816	-2.572874	-1.419069
O	-1.445288	-2.776958	0.118427

O	-1.641961	2.813920	0.168785
O	-1.601754	-1.297036	-2.143194
O	-2.096192	1.324934	-2.039641
O	-1.389890	1.363884	2.438669
O	-1.413828	-1.329976	2.401793
Si	-2.723557	-0.143086	-2.379578
Si	-2.325475	0.028226	2.392304
O	-0.999034	3.944294	2.557932
H	-0.739586	4.789501	2.180927
O	-1.197138	-3.952731	-2.240153
H	-1.219927	-3.878085	-3.198324
O	-0.982186	-3.887920	2.559914
H	-0.709107	-4.735347	2.197843
O	-1.515135	3.932804	-2.213438
H	-1.417180	3.896834	-3.168807
O	-3.278379	0.032533	3.721786
H	-3.379812	-0.819725	4.154641
O	-3.197107	0.103194	1.017510
O	-4.051314	-0.403847	-1.459271
O	-3.141745	-0.235995	-3.960742
H	-3.958733	0.211630	-4.197723
Si	-4.507090	-0.206169	0.103597
O	-5.555784	1.057635	0.084774
H	-5.799138	1.408260	0.946519
O	-5.173005	-1.585942	0.697914
H	-5.887717	-1.969161	0.181917
C	5.575239	-1.434657	0.936722
H	6.139006	-1.833932	0.095878
H	4.825103	-2.076435	1.384579
C	5.965517	-0.277680	1.541844
H	5.525279	0.036459	2.485001
H	6.844535	0.267664	1.219054
H	5.053624	1.222108	0.703115
H	4.166099	0.134547	-2.127294

E_{SCF}= -4479,344286 au

4

Ta	4.049593	0.444599	0.065977
O	2.761189	1.798329	-0.084697
O	3.033115	-1.183880	0.282051
Si	1.111701	1.728043	0.046419
Si	1.401116	-1.342435	0.294004
O	0.720235	0.157288	0.294829
O	0.363561	2.252669	-1.313204
O	0.568755	2.604335	1.319422
O	0.827616	-2.116750	1.625806
O	0.857338	-2.139886	-1.036538
H	5.659773	1.169742	-0.050776
Si	-1.257339	2.614357	-1.393022
Si	-1.054517	2.798766	1.620649
Si	-0.794971	-2.424595	1.803338
Si	-0.753481	-2.486293	-1.225214
O	-1.378048	-2.689146	0.281410
O	-1.768362	2.914603	0.136102
O	-1.444820	-1.234099	-1.999298
O	-2.048935	1.361414	-2.060347
O	-1.619414	1.519738	2.446052
O	-1.546003	-1.165424	2.503913
Si	-2.593311	-0.145568	-2.376761
Si	-2.508289	0.152180	2.387962
O	-1.325645	4.116028	2.538413
H	-1.045956	4.961390	2.176584
O	-0.963749	-3.880520	-2.047491
H	-0.955213	-3.813749	-3.006447
O	-1.042693	-3.699011	2.790300
H	-0.675724	-4.541513	2.508824
O	-1.504853	3.974233	-2.262364
H	-1.385754	3.907356	-3.213591
O	-3.554648	0.154377	3.644470
H	-3.566771	-0.650336	4.169984
O	-3.290311	0.157123	0.958648
O	-3.977664	-0.419929	-1.550092
O	-2.883595	-0.324621	-3.978866
H	-3.707242	0.057612	-4.294440
Si	-4.532196	-0.239458	-0.016343
O	-5.652624	0.956944	-0.108920
H	-5.978257	1.288336	0.733118
O	-5.142887	-1.651542	0.558937
H	-5.820992	-2.072958	0.023694
C	5.944811	-1.549649	-0.390410
H	6.675103	-1.067899	-1.031021
H	5.257378	-2.246965	-0.860635
C	5.964917	-1.380454	0.948157
H	5.294398	-1.936249	1.597377
H	6.711863	-0.757065	1.426950
H	4.772942	0.595569	1.651036
H	4.722049	0.192652	-1.529011

E_{SCF}= -4479,354827 au

TS(3a-5)

Ta	-4.13939	-0.13986	0.33720
O	-2.93444	1.35660	0.16062
O	-2.83473	-1.50498	0.08802
Si	-1.31542	1.51393	0.06461
Si	-1.19783	-1.53768	-0.03501
O	-0.65732	0.01137	-0.05323
O	-0.63923	2.24105	1.37922
O	-0.84208	2.36198	-1.26612
O	-0.69340	-2.26745	-1.41841
O	-0.49358	-2.30507	1.23417
H	-5.09522	-1.45397	1.25902
Si	0.99043	2.54463	1.45531
Si	0.76069	2.67605	-1.56017
Si	0.91860	-2.51622	-1.73462
Si	1.13100	-2.63852	1.28495
O	1.62853	-2.79866	-0.27315
O	1.45358	2.93026	-0.08186
O	1.90101	-1.42739	2.04174
O	1.78932	1.25023	1.99598
O	1.46625	1.43424	-2.33003
O	1.55914	-1.20858	-2.45792
Si	2.68159	-0.04818	2.40581
Si	2.46854	0.14161	-2.29936
O	0.90756	3.97364	-2.54066

H	0.35337	4.73039	-2.33291
O	1.40858	-4.05124	2.05481
H	1.56243	-3.98980	3.00161
O	1.12198	-3.75869	-2.77133
H	0.86109	-4.62765	-2.45427
O	1.30298	3.75518	2.50771
H	0.83352	4.58138	2.36619
O	3.56102	0.24322	-3.51442
H	3.22525	0.12713	-4.40748
O	3.28494	0.12910	-0.90060
O	4.11704	0.01655	1.62116
O	2.92611	-0.09678	4.02272
H	3.25207	0.71585	4.41962
Si	4.60271	0.05093	0.05634
O	5.54207	1.39118	-0.07519
H	5.85298	1.58790	-0.96385
O	5.39271	-1.32935	-0.35389
H	6.11736	-1.58366	0.22431
C	-5.65449	-0.28271	-0.91428
H	-5.68186	-1.18467	0.45589
H	-5.78423	-1.04564	-1.68808
C	-6.71557	0.80102	-0.91761
H	-7.71409	0.39135	-0.72292
H	-6.53791	1.57802	-0.16352
H	-6.73938	1.28804	-1.89945
H	-4.81762	0.60222	1.79653

E_{SCF}= -4479,357541 au

5

Ta	4.12385	-0.18439	-0.33709
O	2.95376	1.32628	-0.25022
O	2.86733	-1.61381	-0.14127
Si	1.33068	1.45578	-0.10154
Si	1.23289	-1.61146	0.00862
O	0.71120	-0.05669	0.07615
O	0.61930	2.13885	-1.41737
O	0.88458	2.32592	1.22068
O	0.71469	-2.36811	1.37236
O	0.50709	-2.33024	-1.27980
H	5.04469	-1.82830	-1.23944
Si	-0.97871	2.58313	-1.44578
Si	-0.70930	2.63169	1.56329
Si	-0.90427	-2.56681	1.68845
Si	-1.13366	-2.56832	-1.33034
O	-1.62978	-2.77965	0.22140
O	-1.45534	2.83687	0.10412
O	-1.82309	-1.26431	-2.00897
O	-1.84323	1.40282	-2.15496
O	-1.36111	1.38719	2.37995
O	-1.49805	-1.25951	2.45167
Si	-2.70415	0.03965	-2.40787
Si	-2.38309	0.11042	2.33299
O	-0.85914	3.94462	2.51958
H	-0.52924	4.77338	2.16152
O	-1.50092	-3.91856	-2.17148
H	-1.65162	-3.79916	-3.11323
O	-1.14827	-3.83126	2.68873
H	-0.88463	-4.69522	2.36054
O	-1.17049	3.99469	-2.24791
H	-0.99833	3.97716	-3.19323
O	-3.46745	0.20120	3.55623
H	-3.13076	0.05454	4.44447
O	-3.21075	0.14456	0.93883
O	-4.10254	0.10400	-1.56098
O	-3.05382	-0.12082	-4.00117
H	-3.76302	0.44092	-4.32591
Si	-4.55203	0.08260	0.01677
O	-5.50716	1.40427	0.20574
H	-5.76348	1.59942	1.11209
O	-5.31513	-1.31985	0.40025
H	-6.10106	-1.52676	-0.11291
C	5.44984	-0.09017	1.06123
H	5.56224	-1.62240	-0.68088
H	5.65037	-0.71169	1.93633
C	6.21498	1.21944	0.99872
H	7.29246	1.04967	0.88446
H	5.91935	1.84854	0.14413
H	6.05407	1.81112	1.90896
H	4.99834	0.33278	-1.79607

E_{SCF}= -4479,363205 au

6

Ta	3.95619	-0.24618	-0.23519
O	3.17213	1.47248	-0.52053
O	2.92084	-1.80258	0.20831
Si	1.53110	1.54804	-0.39141
Si	1.29059	-1.58642	0.23905
O	1.09274	0.03593	0.08923
O	0.77486	1.87637	-1.81231
O	1.00813	2.62030	0.73133
O	0.57791	-2.05277	1.64177
O	0.53060	-2.35963	-0.99530
Si	-0.87140	2.08201	-1.84708
Si	-0.57610	3.09515	0.91511
Si	-1.06720	-2.09558	1.85034
Si	-1.04070	-2.87594	-1.05388
O	-1.67814	-2.73071	0.45233
O	-1.22801	3.09932	-0.60496
O	-1.87278	-1.95415	-2.12722
O	-1.54567	0.61802	-1.51983
O	-1.34613	2.04866	1.88543
O	-1.64635	-0.60750	2.08190
Si	-2.58990	-0.47920	-2.11038
Si	-2.39363	0.84083	2.18057
O	-0.67088	4.56320	1.61170
H	-0.26965	5.29541	1.13577
O	-1.13949	-4.44655	-1.48570
H	-0.88502	-4.66862	-2.38561
O	-1.46823	-2.98555	3.15616
H	-1.15173	-3.89299	3.17799
O	-1.38875	2.65435	-3.27663
H	-1.92891	2.02391	-3.77381
O	-2.97246	1.06105	3.69188
H	-3.19588	0.25811	4.17098

O	-3.58027	0.91706	1.05230
O	-3.94208	-0.56953	-1.20508
O	-2.93360	0.01693	-3.64379
H	-3.75751	-0.28860	-4.03414
Si	-4.61046	-0.00672	0.18799
O	-5.88767	0.89498	-0.30543
H	-6.30295	1.43544	0.37278
O	-5.01702	-1.27429	1.15232
H	-5.29347	-2.07937	0.70589
C	5.57232	-0.21064	0.77524
H	5.67997	-1.27020	1.08691
C	6.64118	0.70011	1.30349
H	6.67507	0.69048	2.40068
H	7.63161	0.38912	0.94706
H	6.48619	1.73552	0.98534
H	4.73995	-0.66734	-1.74074

E_{SCF}= -4478,191783 au

XI. Comparison between cluster and periodic models

XI1. Cluster model

Ethene

C	0.66827	0.00000	0.00000
C	-0.66827	0.00000	0.00000
H	1.24318	0.92988	-0.00001
H	1.24318	-0.92988	0.00002
H	-1.24318	-0.92988	0.00001
H	-1.24318	0.92988	-0.00002

E_{SCF}= -78,4929425 au

Propene

C	0.13033	-0.45564	0.00002
C	1.28684	0.22037	-0.00008
H	0.16191	-1.55268	0.00011
H	1.30905	1.31475	-0.00017
H	2.25083	-0.29321	-0.00009
C	-1.23537	0.16420	0.00005
H	-1.18162	1.26332	-0.00013
H	-1.81555	-0.15299	-0.88348
H	-1.81538	-0.15271	0.88379

E_{SCF}= -117,7657753 au

6

Ta	1.10844	-0.11869	-0.38732
O	0.14300	1.50899	-0.23644
O	-0.06647	-1.58445	-0.00385
Si	-1.48969	1.65738	0.10649
Si	-1.71363	-1.46159	0.22344
O	-2.14735	0.14117	0.19135
O	-2.30859	2.41590	-1.11203
H	-2.06454	3.33617	-1.29202
O	-1.55784	2.45942	1.55062
H	-2.42314	2.51551	1.98298
O	-2.17410	-1.99261	1.72213
H	-1.94932	-2.90905	1.94273
O	-2.40377	-2.30859	-1.01666
H	-3.37089	-2.29951	-1.07312
C	2.79638	-0.25709	0.50510
C	3.95613	0.32643	1.25269
H	2.78940	-1.38357	0.46275
H	4.91454	0.07167	0.76653
H	3.89035	1.42466	1.29194
H	1.73712	-0.32680	-2.02721
H	4.01273	-0.04023	2.29313

E_{SCF}= -1244,7496026 au

21

Ta	0.81167	-0.12478	-0.17053
O	0.24222	1.69223	0.10203
O	-0.15753	-1.78556	-0.07835
Si	-1.44181	1.73935	0.08147
Si	-1.80722	-1.44317	-0.08785
O	-1.88898	0.15829	0.37854
O	-2.00719	2.36429	-1.34293
H	-1.55545	2.00819	-2.12645
O	-2.06657	2.63575	1.31263
H	-2.27280	3.55886	1.10467
O	-2.63896	-2.29608	1.04826
H	-3.03226	-3.12958	0.75074
O	-2.47843	-1.77034	-1.56490
H	-1.94403	-1.44860	-2.31043
C	2.69276	-0.36615	-0.73808
C	3.86873	0.53100	-0.99829
H	2.91734	-1.43996	-0.90646
H	4.18154	0.44559	-2.05436
H	3.64796	1.59144	-0.80224
H	-0.12628	0.06501	-1.73968
H	4.74795	0.24332	-0.39259
C	2.41054	-0.44683	1.78508
H	2.86695	-1.43697	1.72666
H	3.11139	0.39101	1.79199
C	1.09444	-0.28561	2.21344
H	0.75528	0.68689	2.57749
H	0.50127	-1.15548	2.50360

E_{SCF}= -1323,2573658 au

TS(21-22)

Ta	0.79682	-0.12471	-0.16976
O	0.23562	1.69688	0.07908
O	-0.16160	-1.79101	-0.07845
Si	-1.45033	1.73275	0.09219
Si	-1.81137	-1.44257	-0.06377
O	-1.87721	0.15294	0.43163
O	-2.05159	2.32925	-1.33007
H	-1.62276	1.94616	-2.11408
O	-2.05238	2.65051	1.31880
H	-2.28702	3.56201	1.09076
O	-2.63120	-2.31173	1.06857
H	-3.04581	-3.12946	0.75657

O	-2.50436	-1.74629	-1.53624
H	-1.97959	-1.40035	-2.27833
C	2.70686	-0.37183	-0.68247
C	3.86583	0.54294	-0.96948
H	2.94788	-1.44116	-0.84484
H	4.13006	0.46910	-2.03895
H	3.63647	1.59851	-0.75781
H	-0.22696	0.06118	-1.70515
H	4.77257	0.26303	-0.40352
C	2.51799	-0.42716	1.60797
H	2.99731	-1.40849	1.60615
H	3.20990	0.41699	1.65822
C	1.19764	-0.28466	2.10663
H	0.90415	0.67166	2.54647
H	0.67184	-1.16775	2.47673

E_{SCF}= -1323,2572331 au

22

Ta	0.77141	-0.15889	-0.20620
O	0.26995	1.68752	-0.02767
O	-0.21016	-1.80717	-0.10970
Si	-1.41646	1.74843	0.08231
Si	-1.85176	-1.41274	0.00051
O	-1.88064	0.19065	0.47443
O	-2.08198	2.34424	-1.31248
H	-1.72038	1.93388	-2.11566
O	-1.92547	2.70084	1.32481
H	-2.11678	3.62344	1.10103
O	-2.61505	-2.25215	1.19318
H	-3.03370	-3.08308	0.92453
O	-2.63686	-1.73653	-1.42176
H	-2.16327	-1.40620	-2.20341
C	2.82523	-0.44732	-0.29019
C	3.92217	0.41839	-0.89601
H	3.02216	-1.52393	-0.44986
H	4.03208	0.20419	-1.96986
H	3.69662	1.49174	-0.79239
H	-0.39631	0.03813	-1.64648
H	4.90168	0.23653	-0.41841
C	2.65500	-0.21254	1.33329
H	3.24371	-1.01227	1.79998
H	3.11568	0.76306	1.53706
C	1.19852	-0.23355	1.89527
H	0.96100	0.63844	2.51194
H	0.93597	-1.17395	2.39405

E_{SCF}= -1323,2646183 au

TS(22-23)

Ta	-0.81630	-0.14662	-0.06983
O	-0.07469	1.55341	-0.38080
O	0.27883	-1.68566	-0.11628
Si	1.60634	1.67849	-0.10135
Si	1.93661	-1.40533	0.14910
O	2.21609	0.15533	-0.35333
O	1.85905	2.31595	1.40176
H	1.34263	1.82396	2.06952
O	2.31529	2.65212	-1.21952
H	2.31713	3.59997	-1.02062
O	2.86241	-2.36650	-0.81051
H	3.06025	-3.24984	-0.46628
O	2.30038	-1.71749	1.73081
H	1.67467	-1.25334	2.32027
C	-2.72278	-0.30291	0.74284
C	-3.43972	0.70468	1.62948
H	-2.86866	-1.34025	1.09652
H	-3.09941	0.60737	2.67116
H	-3.24093	1.74102	1.31191
H	0.20100	0.09607	1.60654
H	-4.53461	0.55855	1.61575
C	-3.13143	-0.22668	-0.81934
H	-3.89196	-1.00306	-0.97479
H	-3.57783	0.76538	-0.97510
C	-1.95524	-0.44027	-1.86669
H	-1.98162	0.31596	-2.65925
H	-1.97610	-1.44863	-2.30132

E_{SCF}= -1323,2590160 au

23

Ta	-0.95552	-0.20168	-0.02421
O	0.53199	-1.45060	0.16690
O	0.12495	1.34579	-0.13360
Si	2.17338	-1.37598	-0.01286
Si	1.76275	1.67717	-0.08961
O	2.55447	0.23021	-0.24124
O	2.66903	-2.30387	-1.29832
H	1.99639	-2.46414	-1.97753
O	3.02542	-1.85903	1.31603
H	3.17661	-2.81211	1.39878
O	2.00211	2.43584	1.35417
H	2.87815	2.81977	1.50771
O	2.25114	2.69075	-1.30094
H	2.49911	2.27408	-2.13975
C	-2.91596	0.51065	-0.59073
C	-4.03796	-0.33292	-1.18172
H	-2.83477	1.48558	-1.10113
H	-3.85757	-0.51783	-2.25182
H	-4.11027	-1.32099	-0.69617
H	-1.19514	-1.13479	-1.49880
H	-5.02768	0.15182	-1.08426
C	-3.01001	0.69876	0.97210
H	-2.64956	1.68735	1.29989
H	-4.06968	0.63295	1.26958
C	-2.18193	-0.44633	1.66811
H	-2.75151	-1.39021	1.69559
H	-1.80505	-0.19916	2.66907

E_{SCF}= -1323,2862899 au

TS(23-24)

Ta	1.00477	-0.25870	-0.21753
O	-0.51500	-1.43823	-0.05633
O	-0.14213	1.28978	0.07058
Si	-2.17029	-1.35751	0.03893
Si	-1.75007	1.67029	0.22927
O	-2.55695	0.22112	0.37660

O	-2.71531	-2.39759	1.21077
H	-2.08791	-2.60824	1.91785
O	-2.94861	-1.72760	-1.36918
H	-3.02705	-2.66970	-1.58034
O	-2.15436	2.52933	-1.11970
H	-3.02901	2.94556	-1.12535
O	-2.10275	2.59006	1.56305
H	-2.33119	2.10176	2.36788
C	2.61424	0.31563	0.98061
C	3.52593	-0.54823	1.83897
H	2.35966	1.26558	1.48243
H	3.05320	-0.75611	2.81134
H	3.73086	-1.51082	1.34841
H	1.99598	-1.78251	-0.53658
H	4.48912	-0.04716	2.04262
C	3.20948	0.65697	-0.48706
H	3.57434	1.69017	-0.43494
H	4.03251	-0.04557	-0.65418
C	2.20949	0.56321	-1.71747
H	2.58830	-0.08670	-2.51216
H	1.91357	1.54941	-2.09848

E_{SCF}= -1323,2795561 au

24

Ta	-1.02331	0.03046	-0.17577
O	0.35858	1.41205	0.01795
O	0.24221	-1.34386	0.15899
Si	2.00930	1.49351	-0.02872
Si	1.89225	-1.55944	0.18577
O	2.56681	-0.04609	0.27409
O	2.55452	2.57754	1.10574
H	2.01999	2.65203	1.90990
O	2.66492	1.92109	-1.48282
H	2.56014	2.84655	-1.74825
O	2.26470	-2.39526	-1.18466
H	3.16837	-2.73670	-1.25589
O	2.40952	-2.44457	1.48740
H	2.61328	-1.94307	2.29064
C	-2.60153	0.35157	1.15012
C	-3.00921	1.63120	0.43899
H	-2.63093	0.35697	2.24161
H	-2.76316	2.52325	1.02987
H	-2.46636	1.76208	-0.55396
H	-1.18808	0.79766	-1.75184
H	-4.07004	1.65579	0.13457
C	-3.22749	-0.93078	0.47410
H	-3.08713	-1.78565	1.15065
H	-4.30947	-0.75208	0.35268
C	-2.60346	-1.21389	-0.95093
H	-3.25497	-0.87932	-1.76610
H	-2.35148	-2.27369	-1.08820

E_{SCF}= -1323,2890918 au

TS(24-25)

Ta	-0.85936	-0.37639	-0.37282
O	-0.25533	1.52938	-0.26742
O	0.31433	-1.69327	0.25585
Si	1.38703	1.74249	-0.27312
Si	1.95432	-1.29764	0.44209
O	2.08235	0.34948	0.35838
O	1.74693	3.04737	0.69644
H	1.07158	3.24693	1.36224
O	2.14131	2.00421	-1.72059
H	2.10467	2.91612	-2.04527
O	2.72940	-2.15438	-0.72714
H	3.69517	-2.19744	-0.66628
O	2.52317	-1.78361	1.91949
H	2.49139	-1.11712	2.62205
C	-2.07344	0.21006	1.29972
C	-2.18877	1.50720	2.06437
H	-2.00841	-0.67465	1.96688
H	-1.42620	1.55437	2.85823
H	-2.01247	2.35846	1.38508
H	0.23188	-0.12615	-1.79922
H	-3.17258	1.64874	2.54837
C	-3.21470	-0.04261	0.22995
H	-4.01668	-0.63453	0.69373
H	-3.60783	0.94108	-0.06317
C	-2.76396	-0.81718	-1.10095
H	-3.15211	-0.32802	-2.00280
H	-3.05607	-1.87788	-1.08844

E_{SCF}= -1323,2526236 au

25

Ta	-0.82741	-0.26908	-0.51303
O	-0.37126	1.60510	-0.49072
O	0.12640	-1.85984	0.01026
Si	1.27170	1.72115	-0.15673
Si	1.72020	-1.40076	0.33492
O	1.69790	0.25844	0.57061
O	1.61084	2.90714	0.95368
H	1.45757	2.67692	1.88217
O	2.08855	2.11817	-1.52969
H	2.93070	2.57756	-1.39251
O	2.82879	-1.78469	-0.82222
H	3.27347	-2.63647	-0.69594
O	2.21147	-2.16657	1.72478
H	1.52594	-2.33887	2.38674
C	-1.63271	-0.01774	1.46880
C	-1.42566	1.14241	2.42203
H	-1.56338	-0.99199	1.98215
H	-0.47797	1.02605	2.97354
H	-1.38861	2.09636	1.87119
H	0.58621	-0.22339	-1.63619
H	-2.22927	1.21778	3.17723
C	-2.97337	0.04245	0.63364
H	-3.72754	-0.56977	1.14678
H	-3.31183	1.08770	0.60233
C	-2.87448	-0.50210	-0.88014
H	-3.41187	0.15462	-1.57546
H	-3.25303	-1.53137	-0.96525

E_{SCF}= -1323,2599586 au

TS(25-26)

Ta	-0.85031	-0.19764	-0.53697
O	-0.25162	1.62799	-0.47065
O	0.00549	-1.80888	0.08760
Si	1.40336	1.66256	-0.14755
Si	1.63362	-1.49845	0.38637
O	1.72086	0.16490	0.52009
O	1.71821	2.88098	0.93336
H	1.02049	3.07633	1.57651
O	2.38248	1.91773	-1.44357
H	2.65346	2.83732	-1.58391
O	2.68391	-2.02140	-0.76554
H	3.07256	-2.89519	-0.61050
O	2.08302	-2.23248	1.80448
H	1.42501	-2.26567	2.51387
C	-1.71759	0.05949	1.69303
C	-1.51934	1.42626	2.31841
H	-1.22785	-0.77672	2.20372
H	-0.46666	1.58575	2.60195
H	-1.81546	2.23621	1.63414
H	0.41200	-0.31024	-1.81084
H	-2.11841	1.52706	3.24048
C	-2.90168	-0.26032	0.99117
H	-3.28119	-1.28331	0.99879
H	-3.66031	0.50880	0.82464
C	-2.65636	-0.44538	-1.32032
H	-3.27186	0.39233	-1.68317
H	-3.15611	-1.41332	-1.47036

E_{SCF}= -1323,2439053 au

26

Ta	1.32344	-0.00685	-0.16417
O	0.25610	1.55985	-0.07791
O	0.24695	-1.56356	-0.00659
Si	-1.41459	1.57505	0.04636
Si	-1.42635	-1.56512	0.06028
O	-1.95296	0.00700	0.04058
O	-2.12613	2.27823	-1.26839
H	-1.93118	3.21504	-1.42128
O	-1.73662	2.34542	1.47106
H	-2.65528	2.34455	1.77887
O	-1.98788	-2.19041	1.48326
H	-1.74259	-3.10586	1.68538
O	-1.91637	-2.40178	-1.27605
H	-2.86901	-2.45097	-1.44545
C	2.87466	0.01396	0.98102
H	3.32811	-0.89816	1.39992
H	2.19251	-0.03926	-1.70227
H	3.32687	0.93411	1.38242

E_{SCF}= -1205,4806579 au

XI2. Periodic model (xyz coordinates from CONTCAR files)

Ethene

C	1.36554	1.88229	0.85728
C	1.26602	1.94788	2.18689
H	1.05026	2.70484	0.21722
H	1.76605	1.00321	0.35591
H	0.86551	2.82695	2.68826
H	1.58130	1.12533	2.82695

E= -31,965473 eV

Propene

C	2.69522	2.28338	2.42542
C	3.16815	3.10825	3.59315
C	4.45794	3.34012	3.89304
H	3.17487	1.30155	2.40576
H	2.93964	2.77261	1.46997
H	1.60097	2.13003	2.44715
H	2.38385	3.55350	4.21845
H	5.26830	2.91324	3.28951
H	4.75292	3.96428	4.73360

E= -48,578173 eV

6

H	4.11181	10.09063	8.42656
H	2.45388	8.57821	8.20780
H	0.02282	9.04371	8.37526
H	0.98248	2.37899	6.61586
H	5.27477	3.24052	8.31124
H	6.34168	10.80648	1.64724
H	8.91498	11.18210	1.66245
H	4.19475	4.42929	0.68830
H	2.18546	5.83595	0.77635
H	8.74022	1.51398	1.75476
H	7.34117	5.91486	1.78286
H	10.84835	13.97842	1.12478
H	12.46823	4.14421	0.93702
H	6.20402	1.33757	1.66237
H	6.13575	3.99039	2.98100
H	10.41525	9.46124	0.81358
H	11.29970	6.34014	0.61188
H	0.13159	12.70856	34.89639
H	4.53209	11.81724	1.37695
H	2.18809	0.80219	8.32132
H	11.33097	6.36243	10.44469
H	9.20827	8.19348	11.53051
H	7.15483	7.17056	12.75350
H	8.66756	6.79050	13.60776
H	7.88754	5.57164	12.58155
C	8.93363	7.11482	11.49423
C	8.11972	6.63750	12.65980
O	4.39763	11.35759	5.66326
O	7.24339	10.79847	2.07917
O	9.91575	11.19848	1.68897
O	4.66921	3.57386	0.64188
O	1.83338	10.61309	5.81458
O	3.09386	5.86175	1.13484
O	4.99408	13.31698	7.30381
O	10.18374	12.35811	4.13370
O	8.62032	2.86555	4.37118
O	2.57255	4.45239	4.55734
O	5.09947	4.61767	5.45294
O	4.60322	10.84525	1.31565

O	9.92825	6.76041	2.94069
O	7.93735	2.09293	1.87455
O	6.15139	8.72002	3.39893
O	3.15560	10.34865	3.51998
O	3.64394	8.39553	1.74303
O	2.68915	6.53715	6.17658
O	2.24374	6.86207	3.49577
O	3.82558	8.80257	5.54932
O	7.16079	5.10153	6.96186
O	8.79822	9.05369	3.30704
O	9.89495	8.27947	8.67743
O	10.83131	8.68303	6.18299
O	8.22977	9.07100	6.73698
O	7.35712	10.67123	4.74504
O	1.95901	10.21701	1.11122
O	7.22526	6.86988	1.93593
O	9.24578	11.45589	6.46987
O	6.83864	6.51293	4.69478
O	9.63578	1.25600	6.20867
O	9.33006	6.59367	6.71353
O	4.80935	6.43011	3.04300
O	5.24708	6.91907	6.80484
O	9.01519	5.15400	8.91653
O	6.64123	11.20890	7.18512
O	2.35022	1.34374	7.53339
O	4.22030	11.05861	8.36450
O	3.39684	8.26953	8.14043
O	0.23872	8.59792	5.32609
O	11.72473	5.08678	3.78983
O	0.37098	5.95820	5.10770
O	1.52932	12.51158	2.16212
O	11.75925	12.36549	6.30011
O	12.29054	12.07433	2.44451
O	0.78368	9.36865	7.85599
O	11.38405	8.90684	3.53914
O	10.33608	13.81602	1.94938
O	0.37764	2.94104	6.08212
O	0.16972	1.69223	1.11274
O	1.02758	1.75543	3.75421
O	3.80736	2.34147	5.66850
O	2.73350	2.07996	1.75027
O	4.58795	3.21598	3.29043
O	9.53495	3.89863	6.63327
O	11.27104	2.77602	4.90299
O	5.22024	1.17295	1.64027
O	7.04064	4.35032	2.78455
O	9.62169	4.21120	2.30440
O	4.33934	2.96118	8.26257
O	10.37811	8.52337	1.07380
O	11.60577	5.62213	1.19149
O	12.54497	13.31298	0.11631
Si	8.76744	5.16312	7.28368
Si	1.98478	5.93856	4.83515
Si	3.91573	1.79536	7.20468
Si	10.10586	8.34297	2.67833
Si	7.37003	9.80956	3.37493
Si	3.29920	10.27917	5.13265
Si	10.69906	5.40206	2.57415
Si	9.75990	2.72402	5.53048
Si	10.21515	12.55054	5.75901
Si	5.06868	11.70675	7.12898
Si	3.35070	9.96431	1.95202
Si	3.41953	6.92004	2.35482
Si	9.56189	8.17337	7.06051
Si	7.85911	10.59853	6.29099
Si	6.08151	5.80196	5.95670
Si	6.30193	7.10278	3.25814
Si	3.78379	7.63397	6.68045
Si	0.46930	9.86697	6.30410
Si	1.35080	1.37206	2.21191
Si	10.67464	12.33257	2.58528
Si	0.77013	11.26580	1.44870
Si	11.98790	8.78290	5.03838
Si	12.43154	3.91250	4.66770
Si	4.30215	2.51082	1.80905
Si	8.32524	3.35467	2.83948
Si	3.99517	3.65728	4.75390
Ta	9.71849	6.71043	9.78496

E= -814,627046 eV

21

H	4.11364	10.06628	8.42200
H	2.45332	8.55888	8.20687
H	0.01903	9.00236	8.37991
H	1.00299	2.40275	6.58717
H	5.35228	3.26346	8.23724
H	6.30969	10.79332	1.67889
H	8.84934	11.23681	1.68382
H	4.20367	4.40222	0.70293
H	2.30366	5.95325	0.66014
H	8.77356	1.53589	1.76731
H	7.34684	5.91675	1.77597
H	10.90658	1.34128	1.17034
H	12.46169	4.12253	0.89832
H	6.21721	1.31696	1.66863
H	6.11998	3.97458	2.96378
H	10.36228	9.52743	0.81444
H	11.30770	6.32667	0.57378
H	0.19949	12.50837	34.68785
H	4.53688	11.83082	1.41033
H	2.16698	1.00256	8.43946
H	11.30341	6.18162	8.88489
H	10.76743	7.83737	11.64023
H	9.87502	6.46353	13.59230
H	11.47508	5.88533	13.09064
H	10.00514	4.99182	12.61139
H	8.02026	8.43109	11.58608
H	7.52784	6.67216	11.78361
H	7.24201	8.38441	9.20775
H	6.73800	6.61708	9.40953
C	10.35022	6.81821	11.51134
C	10.42212	5.99496	12.75388
C	7.26423	7.48184	9.81008
C	7.68988	7.51117	11.11099

O	4.38725	11.35248	5.68758
O	7.21918	10.77607	2.09653
O	9.85076	11.27384	1.66660
O	4.66241	3.53922	0.64255
O	1.82801	10.59310	5.82795
O	3.15561	5.87248	1.12927
O	4.96292	13.31539	7.33540
O	10.19865	12.37967	4.12631
O	8.61614	2.90743	4.38925
O	2.57636	4.44233	4.53532
O	5.09671	4.59880	5.43957
O	4.60017	10.85887	1.33185
O	9.95845	6.78587	2.91113
O	7.95516	2.08866	1.89779
O	6.17868	8.69142	3.45232
O	3.15800	10.35338	3.53570
O	3.70924	8.39581	1.77578
O	2.68762	6.52107	6.16727
O	2.26776	6.85853	3.48778
O	3.82774	8.79359	5.55508
O	7.12913	5.04314	6.99608
O	8.82105	9.07349	3.32041
O	9.99848	8.39063	8.67402
O	10.77496	8.61435	6.09459
O	8.22842	9.10914	6.77968
O	7.35662	10.67644	4.75754
O	1.97141	10.15063	1.12465
O	7.24458	6.86781	1.95719
O	9.25213	11.48078	6.46333
O	6.87286	6.47168	4.71976
O	9.63860	1.27691	6.20483
O	9.23108	6.61696	6.87111
O	4.83550	6.40692	3.07585
O	5.24603	6.89685	6.80093
O	8.95006	5.07488	8.99885
O	6.64632	11.24836	7.19223
O	2.35004	1.43306	7.58978
O	4.24286	11.03332	8.39031
O	3.39564	8.24849	8.13816
O	0.21014	8.58288	5.36614
O	11.74313	5.08828	3.75015
O	0.37402	5.95508	5.07417
O	1.49415	12.46632	2.09625
O	11.76320	12.37949	6.30091
O	12.26726	12.03000	2.39664
O	0.77225	9.37349	7.88027
O	11.41524	8.93416	3.50116
O	10.39254	13.87618	1.98089
O	0.43122	2.96227	6.01780
O	0.16604	1.66734	1.05053
O	0.99802	1.70980	3.69879
O	3.80382	2.33065	5.67483
O	2.73823	2.01096	1.72597
O	4.57401	3.17366	3.28605
O	9.53390	3.92106	6.65493
O	11.26694	2.80642	4.91542
O	5.23567	1.14164	1.63779
O	7.02120	4.34264	2.76993
O	9.60600	4.23581	2.30263
O	4.41151	2.99520	8.24865
O	10.35675	8.58367	1.05688
O	11.60018	5.60738	1.15716
O	12.55416	13.17288	0.03815
Si	8.73224	5.13229	7.36795
Si	1.98853	5.92763	4.81874
Si	3.92307	1.82306	7.22308
Si	10.12096	8.37160	2.66205
Si	7.37768	9.79946	3.39685
Si	3.29566	10.27115	5.14842
Si	10.70487	5.41327	2.54977
Si	9.75927	2.75551	5.54583
Si	10.22280	12.57460	5.75148
Si	5.06094	11.70938	7.14893
Si	3.36664	9.95590	1.97301
Si	3.46296	6.91545	2.36773
Si	9.56298	8.20328	7.08898
Si	7.86272	10.62652	6.30176
Si	6.08552	5.76621	5.96823
Si	6.33037	7.07707	3.29025
Si	3.78246	7.61437	6.67478
Si	0.45816	9.86161	6.32425
Si	1.33087	1.32825	2.15781
Si	10.66812	12.35969	2.56960
Si	0.76348	11.19519	1.40346
Si	11.98003	8.77083	5.01361
Si	12.44314	3.91351	4.63247
Si	4.29805	2.46787	1.80387
Si	8.32216	3.36823	2.84939
Si	3.99020	3.63798	4.74514
Ta	9.76857	6.71945	9.63579

E= -846,809654 eV

TS(21-22)

H	4.12470	10.06435	8.42326
H	2.45424	8.55705	8.20533
H	0.02097	8.97557	8.36915
H	1.01019	2.39787	6.58287
H	5.34836	3.29185	8.20312
H	6.31357	10.79292	1.68253
H	8.85352	11.24542	1.68769
H	4.21620	4.40412	0.70286
H	2.31999	5.95163	0.66200
H	8.78073	1.53752	1.76629
H	7.35262	5.91916	1.78682
H	10.92297	1.36271	1.18691
H	12.46473	4.11651	0.89373
H	6.22051	1.31478	1.66594
H	6.12684	3.97517	2.96240
H	10.35741	9.53498	0.80797
H	11.30967	6.31546	0.56246
H	0.21269	12.49250	34.67459
H	4.54148	11.83057	1.41484
H	2.17738	0.97698	8.42716
H	11.21866	6.19030	8.79007

H	10.37322	7.95696	11.78970
H	9.37903	6.54476	13.64030
H	10.98742	5.94397	13.18440
H	9.52190	5.09773	12.61888
H	8.00973	8.39925	11.70563
H	7.53274	6.64442	11.82838
H	7.33004	8.41914	9.32173
H	6.80047	6.66820	9.47101
C	9.98431	6.94389	11.58862
C	9.95133	6.08657	12.81479
C	7.46244	7.46356	9.81815
C	7.86607	7.45733	11.18414
O	4.39583	11.34583	5.68946
O	7.22394	10.77519	2.09840
O	9.85470	11.28438	1.66608
O	4.67180	3.53961	0.64008
O	1.83776	10.58146	5.83247
O	3.17034	5.87009	1.13387
O	4.96569	13.31418	7.33363
O	10.20987	12.37923	4.12880
O	8.62267	2.90621	4.38805
O	2.58271	4.44320	4.52983
O	5.10157	4.59536	5.44009
O	4.60644	10.85881	1.33513
O	9.96638	6.78867	2.90314
O	7.96246	2.09028	1.89494
O	6.18774	8.69336	3.46468
O	3.16624	10.34607	3.53942
O	3.72401	8.39293	1.77636
O	2.68912	6.51821	6.16825
O	2.27491	6.86153	3.48800
O	3.83884	8.78574	5.55843
O	7.13092	5.03050	7.00068
O	8.83051	9.07734	3.32015
O	10.03165	8.40526	8.66333
O	10.76698	8.59826	6.07029
O	8.23531	9.11333	6.78081
O	7.36885	10.68292	4.75887
O	1.98044	10.14200	1.12823
O	7.25066	6.87043	1.96797
O	9.26372	11.48303	6.46793
O	6.88029	6.47026	4.72990
O	9.64815	1.27881	6.20564
O	9.22036	6.61817	6.89274
O	4.84317	6.40803	3.08716
O	5.24794	6.88823	6.80829
O	8.95260	5.05782	9.00865
O	6.65661	11.25491	7.19309
O	2.35571	1.43039	7.58886
O	4.25249	11.03158	8.39183
O	3.39608	8.24418	8.14084
O	0.20458	8.58025	5.36670
O	11.75279	5.09056	3.74542
O	0.37873	5.95402	5.06706
O	1.50635	12.46352	2.08717
O	11.77444	12.38276	6.30284
O	12.27543	12.03111	2.39572
O	0.77287	9.36484	7.88119
O	11.42656	8.93438	3.48690
O	10.40476	13.88480	1.99095
O	0.44625	2.96111	6.00977
O	0.17099	1.66135	1.04351
O	1.00086	1.70492	3.69086
O	3.80631	2.32816	5.66933
O	2.74281	2.01364	1.72014
O	4.58003	3.17382	3.28266
O	9.53897	3.92182	6.65504
O	11.27245	2.81077	4.91410
O	5.23896	1.14055	1.63496
O	7.02827	4.34324	2.76976
O	9.61300	4.23708	2.30277
O	4.41585	2.99779	8.24000
O	10.35178	8.59070	1.04803
O	11.60771	5.60430	1.15287
O	12.56592	13.16085	0.03268
Si	8.73303	5.12488	7.37685
Si	1.99359	5.92742	4.81667
Si	3.92740	1.82258	7.21821
Si	10.12637	8.37497	2.65414
Si	7.38617	9.80185	3.40066
Si	3.30580	10.26231	5.15184
Si	10.71253	5.41492	2.54659
Si	9.76547	2.75714	5.54552
Si	10.23334	12.57634	5.75370
Si	5.06946	11.70834	7.14939
Si	3.37644	9.95147	1.97626
Si	3.47380	6.91460	2.37203
Si	9.56785	8.20502	7.08653
Si	7.87285	10.63038	6.30407
Si	6.09039	5.76103	5.97512
Si	6.33769	7.07909	3.30192
Si	3.78659	7.60782	6.67940
Si	0.46311	9.85649	6.32492
Si	1.33749	1.32496	2.15045
Si	10.67737	12.36455	2.57118
Si	0.77377	11.18970	1.40029
Si	11.98138	8.76687	5.00288
Si	12.45092	3.91384	4.62721
Si	4.30338	2.46856	1.80039
Si	8.32917	3.36870	2.84870
Si	3.99518	3.63720	4.74179
Ta	9.69930	6.74525	9.61656

E= -846,763217 eV

22

H	4.13084	10.06393	8.42313
H	2.46160	8.55178	8.20014
H	0.02340	8.98676	8.37164
H	1.01149	2.40159	6.56681
H	5.35828	3.31541	8.16319
H	6.31615	10.80290	1.70882
H	8.84321	11.26044	1.70371
H	4.21345	4.40483	0.69134
H	2.33312	5.97623	0.63750

H	8.78314	1.53628	1.74663
H	7.35596	5.91742	1.77421
H	10.94650	1.40482	1.21817
H	12.46580	4.10801	0.88181
H	6.22272	1.31703	1.64672
H	6.12983	3.96984	2.94921
H	10.35389	9.56787	0.81832
H	11.31543	6.30666	0.53485
H	0.23318	12.45708	34.63513
H	4.54656	11.83428	1.40794
H	2.18521	0.97140	8.41266
H	11.11045	6.12600	8.58431
H	10.05953	7.81030	12.00922
H	9.30995	5.98156	13.65057
H	10.90342	5.64094	12.91826
H	9.44112	4.80369	12.33502
H	7.73999	7.99655	11.92096
H	7.48089	6.24484	11.70784
H	7.46075	8.40513	9.60397
H	6.80953	6.73183	9.49843
C	9.61397	6.86172	11.67368
C	9.82607	5.76484	12.69761
C	7.64440	7.35795	9.83572
C	8.02053	7.12096	11.33214
O	4.40741	11.33988	5.69290
O	7.22375	10.79000	2.13092
O	9.84394	11.30602	1.66321
O	4.66739	3.53963	0.62560
O	1.84603	10.57841	5.83209
O	3.17346	5.87698	1.12312
O	4.96285	13.31480	7.33351
O	10.21857	12.37574	4.12999
O	8.62806	2.88952	4.36432
O	2.58139	4.43990	4.52128
O	5.10031	4.59240	5.42575
O	4.61380	10.86210	1.33514
O	9.97960	6.79076	2.87434
O	7.96679	2.09192	1.86793
O	6.19300	8.68670	3.46251
O	3.17627	10.34799	3.54056
O	3.73588	8.39505	1.77812
O	2.69604	6.51269	6.16197
O	2.28021	6.86029	3.48256
O	3.84531	8.78136	5.55715
O	7.12782	5.00869	6.98920
O	8.83526	9.07116	3.31798
O	10.10389	8.36238	8.67487
O	10.76695	8.59107	6.07119
O	8.26092	9.12905	6.84567
O	7.38026	10.65204	4.78893
O	1.98900	10.13543	1.12928
O	7.25533	6.86788	1.95951
O	9.27325	11.49444	6.47646
O	6.88355	6.46160	4.72159
O	9.65883	1.28658	6.19865
O	9.18864	6.62178	6.86862
O	4.84791	6.40166	3.07793
O	5.25442	6.87957	6.80355
O	8.95931	5.01206	8.98916
O	6.66535	11.26549	7.20790
O	2.36011	1.44873	7.58738
O	4.25477	11.03145	8.39357
O	3.40192	8.23417	8.13823
O	0.20361	8.57992	5.37188
O	11.76249	5.08986	3.72190
O	0.38287	5.95505	5.06572
O	1.50532	12.45762	2.07864
O	11.78453	12.38969	6.30247
O	12.27565	12.02654	2.38415
O	0.77857	9.36780	7.88237
O	11.42994	8.93568	3.48907
O	10.41783	13.90019	2.00694
O	0.44252	2.96242	5.99636
O	0.16318	1.65172	1.04259
O	1.01425	1.70553	3.68221
O	3.81049	2.32412	5.65667
O	2.74275	2.00554	1.69904
O	4.57527	3.17009	3.26784
O	9.54724	3.93425	6.61735
O	11.27899	2.80921	4.88946
O	5.24144	1.14102	1.61841
O	7.03087	4.33815	2.75667
O	9.61574	4.23883	2.28824
O	4.43066	3.00860	8.22084
O	10.36025	8.61986	1.04482
O	11.61216	5.59660	1.12675
O	12.57710	13.13887	0.01664
Si	8.73192	5.12019	7.35763
Si	1.99682	5.92575	4.81028
Si	3.93348	1.82881	7.20873
Si	10.13444	8.38011	2.64660
Si	7.39237	9.79517	3.41638
Si	3.31499	10.25960	5.15282
Si	10.72060	5.41364	2.52357
Si	9.77241	2.75803	5.52253
Si	10.24252	12.58167	5.75370
Si	5.07593	11.70930	7.15347
Si	3.38577	9.95309	1.97721
Si	3.47940	6.91514	2.36644
Si	9.58272	8.19279	7.10544
Si	7.88744	10.63049	6.33326
Si	6.09334	5.75209	5.96643
Si	6.34263	7.07285	3.29421
Si	3.79421	7.60083	6.67512
Si	0.46879	9.85806	6.32500
Si	1.33959	1.31916	2.14049
Si	10.68146	12.37276	2.57027
Si	0.77836	11.18101	1.39085
Si	11.98188	8.76569	5.00539
Si	12.45648	3.91435	4.60960
Si	4.30188	2.46633	1.78456
Si	8.33368	3.36520	2.82963
Si	3.99462	3.63386	4.72841
Ta	9.71445	6.69618	9.59414

E= -846,983447 eV

TS(22-23)

H	4.12918	10.06325	8.41768
H	2.45615	8.54824	8.19167
H	0.02276	8.92580	8.33445
H	1.00324	2.39179	6.55320
H	5.35919	3.28624	8.17257
H	6.31708	10.79671	1.67481
H	8.84566	11.24629	1.66420
H	4.20773	4.41028	0.68321
H	2.32172	5.97241	0.62941
H	8.77524	1.52964	1.69734
H	7.35059	5.91052	1.76099
H	10.94356	1.40013	1.21173
H	12.47016	4.11405	0.87343
H	6.22597	1.32547	1.61386
H	6.13140	3.96080	2.93950
H	10.35411	9.54861	0.80217
H	11.32516	6.32328	0.53562
H	0.22971	12.46873	34.62520
H	4.54357	11.83001	1.39988
H	2.18454	0.96343	8.40125
H	11.38514	6.47023	9.18812
H	10.07856	7.65913	12.12237
H	9.29924	5.75079	13.68531
H	10.87044	5.42784	12.89501
H	9.37959	4.65115	12.29994
H	7.75509	7.86901	12.17673
H	7.43142	6.18050	11.71494
H	7.54361	8.65134	9.95047
H	6.77196	7.06527	9.60925
C	9.58439	6.74357	11.76292
C	9.79088	5.58299	12.70979
C	7.65813	7.57303	10.02076
C	8.00593	7.08031	11.46315
O	4.40096	11.33868	5.67960
O	7.22728	10.77905	2.09088
O	9.84651	11.29483	1.62627
O	4.66528	3.54695	0.61706
O	1.84240	10.58099	5.82936
O	3.16400	5.87557	1.11262
O	4.97318	13.30660	7.32012
O	10.21369	12.34154	4.10523
O	8.63799	2.85770	4.31531
O	2.58219	4.43590	4.52442
O	5.11016	4.58435	5.42109
O	4.61057	10.85801	1.32785
O	9.96836	6.78233	2.86970
O	7.96534	2.09655	1.80707
O	6.18703	8.68896	3.43571
O	3.16287	10.34766	3.52906
O	3.72317	8.39242	1.77009
O	2.69078	6.51185	6.15530
O	2.27404	6.85076	3.47556
O	3.83910	8.78026	5.54265
O	7.15158	5.04324	6.96644
O	8.83094	9.07114	3.30190
O	10.02185	8.32900	8.65082
O	10.78048	8.63679	6.07848
O	8.23656	9.08197	6.75838
O	7.36342	10.66614	4.75172
O	1.98828	10.14146	1.10994
O	7.24956	6.86189	1.94119
O	9.26037	11.46399	6.45285
O	6.87809	6.46671	4.70145
O	9.65251	1.25787	6.16282
O	9.28879	6.59811	6.78578
O	4.84243	6.39993	3.06404
O	5.24852	6.88001	6.79103
O	9.02926	5.04222	8.90846
O	6.65993	11.23529	7.18537
O	2.36225	1.43062	7.57068
O	4.25283	11.03070	8.38280
O	3.39910	8.23728	8.12702
O	0.23029	8.57519	5.33206
O	11.74391	5.07314	3.71457
O	0.37533	5.94645	5.05986
O	1.49591	12.45763	2.07265
O	11.77370	12.36176	6.28388
O	12.27254	12.01924	2.36035
O	0.77063	9.34170	7.86185
O	11.42562	8.92297	3.47940
O	10.40781	13.88802	1.99352
O	0.41786	2.94508	5.99157
O	0.16172	1.65640	1.03611
O	1.02675	1.71564	3.67134
O	3.81541	2.31955	5.64937
O	2.74568	1.99993	1.68195
O	4.57109	3.16942	3.25871
O	9.54646	3.90343	6.57081
O	11.28890	2.77518	4.85790
O	5.24471	1.14670	1.60207
O	7.03166	4.32840	2.74203
O	9.61337	4.23610	2.25296
O	4.42688	2.99310	8.21732
O	10.35822	8.60189	1.03467
O	11.61796	5.60698	1.12233
O	12.57580	13.14749	0.00120
Si	8.76527	5.13369	7.26136
Si	1.98981	5.92095	4.80648
Si	3.93569	1.81510	7.19874
Si	10.12925	8.37139	2.63811
Si	7.38772	9.79720	3.38762
Si	3.30685	10.25967	5.14173
Si	10.71433	5.41051	2.50907
Si	9.77725	2.72133	5.47645
Si	10.23350	12.54579	5.72964
Si	5.07682	11.69879	7.13932
Si	3.37842	9.95179	1.96672
Si	3.46998	6.91174	2.35759
Si	9.58387	8.19173	7.09094
Si	7.87382	10.60030	6.29638
Si	6.08921	5.76184	5.94763

Si	6.33603	7.07571	3.27327
Si	3.78710	7.60314	6.66434
Si	0.46850	9.84239	6.30710
Si	1.34156	1.31999	2.12953
Si	10.67691	12.35682	2.54610
Si	0.77489	11.18288	1.37427
Si	11.98260	8.76679	4.99683
Si	12.45252	3.90081	4.59390
Si	4.30222	2.46885	1.77213
Si	8.33483	3.35475	2.78816
Si	3.99668	3.63059	4.72292
Ta	9.61975	6.65787	9.68975

E= -846,782358 eV

23

H	4.13122	10.06263	8.40169
H	2.47296	8.53680	8.16311
H	0.03093	8.96083	8.31216
H	0.99986	2.38342	6.52428
H	5.37553	3.25081	8.18893
H	6.33208	10.81438	1.63697
H	8.84912	11.22596	1.61646
H	4.18907	4.40383	0.64587
H	2.27500	5.96440	0.58276
H	8.77393	1.51892	1.64634
H	7.35407	5.91342	1.69464
H	10.93395	1.35369	1.16370
H	12.48795	4.13227	0.85474
H	6.24507	1.33418	1.56873
H	6.14487	3.96318	2.90089
H	10.36700	9.54404	0.79452
H	11.33822	6.34138	0.52263
H	0.21581	12.51968	34.64214
H	4.55510	11.82609	1.36077
H	2.20403	0.93722	8.36120
H	11.16636	6.94789	10.36627
H	9.71054	6.87971	12.67080
H	9.26220	4.42554	13.29191
H	10.83547	4.65267	12.46985
H	9.43495	3.99884	11.58261
H	7.25460	6.54294	12.62731
H	7.32979	5.50581	11.21766
H	7.92286	8.54208	11.29487
H	6.85466	7.68629	10.11407
C	9.33709	6.14129	11.94885
C	9.73866	4.73624	12.34161
C	7.75676	7.60973	10.74699
C	7.81324	6.38052	11.68597
O	4.40725	11.33923	5.65471
O	7.23787	10.80550	2.06318
O	9.85131	11.26748	1.57891
O	4.66018	3.54759	0.58637
O	1.84724	10.59509	5.79488
O	3.12693	5.87644	1.05172
O	4.99734	13.29766	7.29378
O	10.20551	12.30347	4.06409
O	8.64747	2.83567	4.25458
O	2.58164	4.41962	4.50173
O	5.11035	4.59886	5.37026
O	4.62247	10.85354	1.29853
O	9.94741	6.77084	2.84097
O	7.97061	2.09700	1.74498
O	6.16815	8.70001	3.34323
O	3.17016	10.35139	3.49763
O	3.68486	8.39444	1.72435
O	2.71143	6.50707	6.11653
O	2.26959	6.82940	3.43532
O	3.83902	8.78339	5.50788
O	7.18246	5.06450	6.87239
O	8.81774	9.06463	3.27089
O	9.92210	8.10968	8.57686
O	10.84887	8.67723	6.12657
O	8.25523	9.05962	6.71007
O	7.34352	10.64279	4.72496
O	1.99572	10.18197	1.07345
O	7.24338	6.86530	1.86506
O	9.24974	11.45387	6.41766
O	6.85494	6.49156	4.62264
O	9.65982	1.24248	6.10577
O	9.31388	6.57968	6.48590
O	4.83349	6.39733	2.97426
O	5.26895	6.89031	6.74384
O	9.07991	5.20424	8.75523
O	6.65895	11.19586	7.16676
O	2.38079	1.41310	7.53402
O	4.24767	11.03027	8.35779
O	3.41564	8.22762	8.09405
O	0.27179	8.57352	5.27751
O	11.72987	5.07995	3.70167
O	0.38800	5.93826	5.04819
O	1.46464	12.46593	2.09726
O	11.76910	12.33462	6.24203
O	12.27190	11.99671	2.32573
O	0.78537	9.33639	7.81792
O	11.40476	8.90141	3.48619
O	10.40162	13.85938	1.95444
O	0.38594	2.93241	5.98871
O	0.17191	1.67368	1.02380
O	1.05337	1.76430	3.65496
O	3.83912	2.31872	5.62641
O	2.76217	1.97333	1.64921
O	4.57540	3.16263	3.22668
O	9.56045	3.88575	6.50770
O	11.30108	2.75616	4.79556
O	5.26442	1.14890	1.56645
O	7.04452	4.32804	2.69747
O	9.62672	4.22758	2.20362
O	4.43614	2.97955	8.19910
O	10.37564	8.59549	1.02301
O	11.63327	5.62418	1.10754
O	12.56740	13.18695	34.99638
Si	8.80490	5.17010	7.13124
Si	2.00131	5.91026	4.77563
Si	3.95518	1.80404	7.17281

Si	10.12054	8.35894	2.62083
Si	7.37800	9.79973	3.34463
Si	3.31163	10.26531	5.11061
Si	10.71388	5.40952	2.48160
Si	9.78726	2.70379	5.41511
Si	10.23030	12.52419	5.68638
Si	5.08344	11.68769	7.11716
Si	3.37838	9.95982	1.93333
Si	3.44622	6.90659	2.29703
Si	9.57583	8.11791	6.97643
Si	7.87130	10.58004	6.26346
Si	6.09776	5.77634	5.87991
Si	6.31988	7.08487	3.18930
Si	3.80225	7.60350	6.62680
Si	0.48088	9.83843	6.26469
Si	1.34803	1.33167	2.11871
Si	10.67397	12.32872	2.50642
Si	0.76893	11.19940	1.36157
Si	12.00649	8.76631	4.98570
Si	12.44955	3.90580	4.56930
Si	4.31203	2.46282	1.73949
Si	8.34390	3.34874	2.73346
Si	4.00503	3.62543	4.69103
Ta	9.47707	6.71508	9.86384

E= -847,675908 eV

TS(23-24)

H	4.10153	10.09524	8.37758
H	2.43335	8.55539	8.14178
H	12.59764	10.56254	8.31200
H	1.00982	2.39733	6.51848
H	5.37395	3.34271	8.08305
H	6.30698	10.82715	1.60689
H	8.83683	11.26948	1.60057
H	4.17775	4.40420	0.63696
H	2.31215	6.01133	0.52922
H	8.77110	1.54358	1.74435
H	7.35934	5.92255	1.69944
H	10.92064	1.41420	1.17990
H	12.45496	4.13067	0.85783
H	6.20506	1.31791	1.62543
H	6.11704	3.98825	2.90480
H	10.35908	9.56048	0.75347
H	11.31152	6.32118	0.50949
H	0.20647	12.47540	34.59178
H	4.52552	11.85809	1.37249
H	2.28012	0.76650	8.28333
H	10.13035	8.31443	11.02348
H	11.28141	6.43288	11.98160
H	11.15369	3.91208	12.32026
H	12.02385	4.35906	10.83595
H	10.34065	3.76263	10.73611
H	9.27426	6.49995	13.11854
H	8.75236	4.94489	12.38339
H	7.59892	7.61006	11.89926
H	7.08689	6.05244	11.14260
C	10.54718	5.80369	11.45870
C	11.03390	4.37967	11.32898
C	7.93471	6.70555	11.39411
C	9.10069	5.95962	12.18565
O	4.39489	11.35861	5.62163
O	7.21773	10.80924	2.02113
O	9.83825	11.31401	1.57358
O	4.63925	3.54204	0.58540
O	1.83262	10.61938	5.78631
O	3.14486	5.89855	1.02253
O	5.02588	13.30721	7.25495
O	10.17684	12.34914	4.06399
O	8.60660	2.94343	4.36095
O	2.58572	4.44137	4.48267
O	5.11225	4.61276	5.38866
O	4.58807	10.88663	1.28385
O	9.96369	6.79982	2.83047
O	7.95024	2.09190	1.87526
O	6.17086	8.70976	3.33923
O	3.14471	10.35719	3.48210
O	3.70078	8.41370	1.70366
O	2.69375	6.52644	6.09332
O	2.27450	6.84808	3.40449
O	3.82199	8.80547	5.50025
O	7.17002	5.11169	6.91502
O	8.81606	9.09060	3.23300
O	9.88082	8.08687	8.51446
O	10.84110	8.68791	6.08294
O	8.24491	9.05279	6.63739
O	7.34890	10.67866	4.68222
O	1.96582	10.16350	1.06698
O	7.25599	6.87467	1.87297
O	9.23791	11.46107	6.40696
O	6.84570	6.50799	4.63358
O	9.62834	1.25929	6.13703
O	9.31956	6.57214	6.42184
O	4.83703	6.41032	2.96369
O	5.24481	6.91426	6.74336
O	9.06869	5.43265	8.79730
O	6.64467	11.17301	7.13387
O	2.41786	1.39842	7.56137
O	4.22650	11.06131	8.32347
O	3.37616	8.24493	8.07994
O	0.26197	8.59943	5.25986
O	11.73911	5.09621	3.69763
O	0.38210	5.96372	5.00094
O	1.48006	12.47040	2.04790
O	11.75159	12.36276	6.22831
O	12.25621	12.03122	2.33932
O	0.75812	9.36153	7.80419
O	11.40563	8.94477	3.44702
O	10.39803	13.90570	1.97180
O	0.41986	2.96471	5.97834
O	0.14938	1.67363	1.02083
O	0.98912	1.70760	3.66468
O	3.82799	2.34117	5.62577
O	2.72764	2.01703	1.69374
O	4.58293	3.18340	3.23184

O	9.53268	3.88507	6.66001
O	11.25550	2.81623	4.87711
O	5.22339	1.14714	1.58386
O	7.01960	4.35658	2.71744
O	9.60486	4.24071	2.25652
O	4.46955	2.98620	8.18566
O	10.36942	8.61475	0.98968
O	11.59857	5.60237	1.09586
O	12.53809	13.16673	34.98564
Si	8.79437	5.22846	7.19259
Si	1.99751	5.93133	4.74445
Si	3.97665	1.81084	7.16488
Si	10.12204	8.38642	2.59021
Si	7.37236	9.81746	3.31160
Si	3.29262	10.28307	5.09407
Si	10.70420	5.42025	2.49109
Si	9.74979	2.75156	5.51183
Si	10.20576	12.55190	5.68839
Si	5.08184	11.69633	7.08136
Si	3.35988	9.97231	1.91749
Si	3.45873	6.92524	2.27388
Si	9.56423	8.10957	6.91462
Si	7.86543	10.58207	6.22378
Si	6.09255	5.80071	5.89743
Si	6.32396	7.09355	3.19250
Si	3.77844	7.62334	6.61568
Si	0.46142	9.86397	6.24931
Si	1.31983	1.33159	2.12023
Si	10.65853	12.36858	2.51033
Si	0.75269	11.19977	1.34939
Si	12.00167	8.79309	4.94788
Si	12.43008	3.92024	4.58509
Si	4.28831	2.47529	1.75419
Si	8.31835	3.38177	2.81258
Si	4.00664	3.64841	4.69436
Ta	9.49557	6.91084	10.01647

E= -847,492276 eV

24

H	4.09659	10.09961	8.40332
H	2.40669	8.55684	8.14416
H	12.56442	10.56765	8.29394
H	1.00385	2.38184	6.52878
H	5.34579	3.34886	8.10550
H	6.29902	10.83244	1.64101
H	8.82540	11.26264	1.62235
H	4.15700	4.40358	0.63736
H	2.27584	5.99862	0.55060
H	8.75752	1.54504	1.75278
H	7.35391	5.91750	1.70350
H	10.90420	1.40580	1.17700
H	12.43295	4.12391	0.87158
H	6.18471	1.31817	1.63284
H	6.09960	3.98671	2.91344
H	10.33583	9.53920	0.73620
H	11.29376	6.31250	0.52452
H	0.19556	12.47307	34.60256
H	4.51366	11.85797	1.37561
H	2.25983	0.75693	8.27727
H	9.01344	8.29391	10.65768
H	11.96874	6.96461	11.51881
H	12.33332	4.46841	11.99124
H	0.05756	3.33565	10.28712
H	11.12788	4.08323	10.73633
H	10.07810	7.08806	12.93409
H	10.15445	5.31238	12.92438
H	7.81798	6.73251	12.19512
H	8.19983	5.09380	11.56488
C	11.23004	6.19275	11.25147
C	11.87211	4.83172	11.05654
C	8.55193	6.12582	11.66227
C	10.00081	6.19991	12.30561
O	4.38490	11.35570	5.64133
O	7.20486	10.82367	2.06586
O	9.82668	11.30675	1.58798
O	4.61942	3.54190	0.58817
O	1.81470	10.62929	5.78579
O	3.12540	5.90141	1.02159
O	5.00218	13.31236	7.27006
O	10.15265	12.36118	4.07166
O	8.58382	2.94105	4.37481
O	2.55641	4.43659	4.48133
O	5.07580	4.62074	5.38797
O	4.57735	10.88650	1.28924
O	9.95846	6.80193	2.84950
O	7.93594	2.09217	1.88643
O	6.16005	8.70296	3.33874
O	3.14238	10.36043	3.49209
O	3.69226	8.41521	1.71080
O	2.67214	6.52146	6.09533
O	2.26638	6.84878	3.40685
O	3.79454	8.80593	5.51346
O	7.13064	5.09842	6.91429
O	8.80998	9.08940	3.24558
O	10.02980	8.01886	8.48774
O	10.79812	8.68965	6.02674
O	8.24984	9.06379	6.73472
O	7.33596	10.63570	4.72873
O	1.95176	10.15911	1.08226
O	7.25419	6.86928	1.87986
O	9.22576	11.46719	6.42160
O	6.82145	6.50548	4.63959
O	9.60533	1.26466	6.15480
O	9.26240	6.58076	6.41899
O	4.82781	6.40377	2.95310
O	5.22071	6.91637	6.74908
O	9.04213	5.41504	8.79262
O	6.63272	11.18523	7.16352
O	2.39381	1.40280	7.56762
O	4.20747	11.06624	8.34087
O	3.34505	8.23363	8.09019
O	0.23609	8.61129	5.25417
O	11.72983	5.09311	3.71406
O	0.36309	5.97351	4.99301

O	1.47418	12.46907	2.05403
O	11.73461	12.37692	6.22795
O	12.24219	12.03771	2.35375
O	0.73246	9.36799	7.79894
O	11.40981	8.95615	3.41362
O	10.37986	13.90232	1.96937
O	0.41057	2.95177	5.99385
O	0.13045	1.66721	1.03201
O	0.96934	1.69587	3.67662
O	3.80782	2.34084	5.63017
O	2.70621	2.02302	1.70289
O	4.56280	3.18352	3.23629
O	9.50209	3.89412	6.67011
O	11.23255	2.81837	4.89468
O	5.20305	1.14860	1.58868
O	7.00250	4.35469	2.72739
O	9.58966	4.24214	2.27746
O	4.43878	2.99444	8.19124
O	10.33343	8.59628	0.98103
O	11.58608	5.59839	1.11408
O	12.52762	13.16376	34.99550
Si	8.75035	5.23580	7.19210
Si	1.97908	5.93098	4.74313
Si	3.95429	1.81604	7.17155
Si	10.10960	8.38620	2.58805
Si	7.36302	9.80875	3.33838
Si	3.27996	10.28690	5.10513
Si	10.69233	5.41903	2.51037
Si	9.72547	2.75653	5.52793
Si	10.18446	12.56051	5.69679
Si	5.06823	11.70066	7.10169
Si	3.35063	9.97303	1.92684
Si	3.44732	6.92445	2.27291
Si	9.57312	8.10321	6.92546
Si	7.85736	10.57555	6.27007
Si	6.06141	5.80094	5.90049
Si	6.31259	7.08705	3.19305
Si	3.75240	7.61998	6.62425
Si	0.44132	9.87508	6.24285
Si	1.30314	1.32888	2.13015
Si	10.64257	12.36949	2.51931
Si	0.74107	11.19880	1.36083
Si	11.98487	8.80339	4.92357
Si	12.41528	3.91302	4.60029
Si	4.26824	2.47723	1.75866
Si	8.30158	3.38060	2.82627
Si	3.97992	3.64752	4.69607
Ta	9.68132	6.79999	9.98232

E= -847,676553 eV

TS(24-25)

H	4.14297	10.10621	8.43591
H	2.45257	8.56754	8.16868
H	0.01850	9.00993	8.34924
H	1.06821	2.24608	6.45008
H	5.32113	3.32703	8.14511
H	6.32443	10.82998	1.70356
H	8.87357	11.27940	1.66852
H	4.18906	4.41959	0.63379
H	2.30291	5.98505	0.62403
H	8.74006	1.54832	1.70178
H	7.37931	5.89919	1.72244
H	10.99755	1.62418	1.37198
H	12.36168	4.07740	0.83912
H	6.10617	1.28709	1.60587
H	6.08628	3.96857	2.89699
H	10.39916	9.50671	0.76480
H	11.26560	6.32803	0.52757
H	0.29677	12.07438	34.28772
H	4.51350	11.84432	1.38941
H	2.27041	0.68957	8.23303
H	8.09963	7.54997	9.34886
H	12.46058	7.10675	9.62676
H	0.51000	3.13591	10.19403
H	12.40012	4.83005	8.56577
H	11.42157	4.18940	9.90549
H	11.81895	7.47860	11.82560
H	11.75862	5.71048	12.05976
H	9.54276	7.53441	12.41593
H	9.39191	5.75298	12.33896
C	11.74415	6.35091	9.96469
C	12.19064	4.93894	9.63974
C	9.77200	6.64537	11.82932
C	11.35698	6.54991	11.48338
O	4.42185	11.32601	5.66796
O	7.22898	10.82214	2.12996
O	9.87120	11.33891	1.61355
O	4.63118	3.54736	0.57958
O	1.84424	10.60519	5.81462
O	3.16361	5.89364	1.07301
O	5.03586	13.30829	7.26835
O	10.21940	12.35003	4.09327
O	8.56090	2.87811	4.35705
O	2.55769	4.42181	4.51188
O	5.09058	4.60297	5.37176
O	4.60014	10.87308	1.31524
O	10.03094	6.78762	2.91464
O	7.92320	2.09747	1.83906
O	6.20687	8.67429	3.38673
O	3.16149	10.36297	3.51670
O	3.77638	8.39321	1.77781
O	2.68509	6.50407	6.14014
O	2.30646	6.84123	3.45585
O	3.81533	8.77934	5.52107
O	7.12198	5.02897	6.92846
O	8.84832	9.07151	3.25369
O	10.20093	8.20192	8.62880
O	10.77347	8.60959	6.04703
O	8.28759	9.06522	6.84290
O	7.38712	10.58789	4.78585
O	1.98983	10.05554	1.10987
O	7.30331	6.84931	1.91786
O	9.28335	11.44415	6.44629
O	6.88514	6.47195	4.67732

O	9.61573	1.24188	6.16366
O	9.29328	6.56326	6.75244
O	4.87719	6.37383	3.00516
O	5.24106	6.88795	6.75510
O	8.93890	5.05837	8.91359
O	6.67904	11.20105	7.19474
O	2.40796	1.34602	7.53355
O	4.24754	11.07284	8.36610
O	3.38751	8.23511	8.10818
O	0.23591	8.57707	5.35943
O	11.80668	5.01658	3.65247
O	0.37738	5.95250	5.03101
O	1.56076	12.45315	1.81805
O	11.77602	12.38618	6.26702
O	12.29355	12.10512	2.35640
O	0.77581	9.39659	7.86670
O	11.44710	8.96692	3.46892
O	10.38722	13.94073	2.01128
O	0.46588	2.82077	5.92847
O	0.04297	1.61835	1.01513
O	0.95564	1.52196	3.61241
O	3.82747	2.32118	5.62517
O	2.63897	2.09699	1.64070
O	4.52777	3.16994	3.22045
O	9.52150	3.87610	6.61894
O	11.21490	2.76841	4.83989
O	5.12328	1.13236	1.57088
O	6.99261	4.33708	2.73553
O	9.57954	4.24133	2.30724
O	4.41116	2.97392	8.19780
O	10.40577	8.56873	1.02616
O	11.54551	5.57956	1.07945
O	12.56447	12.92391	34.88521
Si	8.72374	5.12960	7.25937
Si	1.99260	5.91877	4.78426
Si	3.96605	1.79154	7.16526
Si	10.16525	8.37294	2.63458
Si	7.40393	9.78644	3.38322
Si	3.30755	10.26751	5.12876
Si	10.71415	5.39477	2.51099
Si	9.72085	2.71466	5.49514
Si	10.22865	12.54545	5.71747
Si	5.10996	11.69453	7.12076
Si	3.39122	9.94366	1.96168
Si	3.49766	6.90665	2.33146
Si	9.62557	8.14116	7.11060
Si	7.90681	10.55847	6.32741
Si	6.07723	5.76940	5.91187
Si	6.36345	7.06104	3.23388
Si	3.77724	7.60427	6.64514
Si	0.47123	9.86859	6.30193
Si	1.28818	1.28572	2.03605
Si	10.69111	12.40986	2.53345
Si	0.78888	11.12829	1.27789
Si	11.98751	8.77724	4.98993
Si	12.44300	3.80781	4.53754
Si	4.22190	2.48716	1.73525
Si	8.28967	3.35817	2.81681
Si	3.98259	3.63213	4.69521
Ta	9.60081	6.61190	9.75582

E= -846,827464 eV

25

H	4.15773	10.10460	8.43004
H	2.47878	8.58427	8.18926
H	0.02642	9.08833	8.38316
H	1.09260	2.23046	6.41498
H	5.28843	3.29760	8.23108
H	6.34830	10.80881	1.66858
H	8.90980	11.26950	1.65813
H	4.22450	4.42413	0.66009
H	2.32952	5.97364	0.65797
H	8.74535	1.54657	1.73132
H	7.37096	5.90979	1.74711
H	10.97606	1.58273	1.30824
H	12.39828	4.10013	0.80950
H	6.13384	1.29534	1.64660
H	6.10142	3.98848	2.91270
H	10.42854	9.52431	0.80579
H	11.25753	6.34144	0.51677
H	0.30408	12.01563	34.25497
H	4.52772	11.83678	1.40477
H	2.26248	0.66345	8.21332
H	8.03163	7.20523	8.75347
H	12.31150	6.86752	9.03776
H	0.54662	3.01752	9.51546
H	11.99195	4.52074	8.16918
H	11.46408	3.99568	9.78372
H	12.19131	7.33916	11.31334
H	11.88181	5.61481	11.64873
H	10.04334	7.79612	12.17544
H	9.64792	6.05644	12.28540
C	11.66636	6.14060	9.54791
C	12.08785	4.72544	9.24447
C	10.05292	6.84549	11.64192
C	11.54090	6.48702	11.08722
O	4.43046	11.34012	5.66961
O	7.25843	10.78660	2.08173
O	9.90841	11.32544	1.62561
O	4.66455	3.55116	0.60480
O	1.85543	10.62165	5.82000
O	3.18617	5.88471	1.11883
O	5.05542	13.31300	7.28102
O	10.23721	12.37023	4.09441
O	8.56256	2.90055	4.38102
O	2.59809	4.44259	4.54540
O	5.13664	4.60432	5.41960
O	4.61155	10.86625	1.32219
O	10.04065	6.78016	2.91736
O	7.92766	2.09294	1.87546
O	6.21731	8.68831	3.41978
O	3.16630	10.37211	3.52199
O	3.78965	8.38954	1.80298
O	2.69736	6.52318	6.17298

O	2.30764	6.85294	3.48627
O	3.82536	8.79315	5.53272
O	7.17503	5.08485	6.96512
O	8.85983	9.06467	3.27840
O	10.09569	8.38199	8.66373
O	10.81492	8.63797	6.11116
O	8.26914	9.05773	6.74503
O	7.39995	10.65263	4.74207
O	2.00076	10.04302	1.11521
O	7.29197	6.86201	1.93485
O	9.29695	11.44376	6.43744
O	6.91603	6.48439	4.69896
O	9.62415	1.24831	6.17045
O	9.44094	6.54499	6.79769
O	4.88146	6.38597	3.06351
O	5.26188	6.90853	6.76642
O	8.99233	5.03610	8.97901
O	6.69325	11.20181	7.17787
O	2.40988	1.30726	7.50403
O	4.27288	11.07153	8.36984
O	3.41566	8.25942	8.12506
O	0.26074	8.58507	5.37414
O	11.83781	5.01264	3.62072
O	0.39436	5.95361	5.06876
O	1.59545	12.46087	1.75861
O	11.78552	12.39260	6.27503
O	12.31933	12.13107	2.36772
O	0.79412	9.42425	7.87968
O	11.45127	8.95598	3.50942
O	10.39323	13.93757	1.99453
O	0.50875	2.81514	5.88450
O	0.09252	1.64248	0.96546
O	0.93585	1.47841	3.58163
O	3.85164	2.33186	5.64372
O	2.66936	2.11274	1.67695
O	4.56044	3.19308	3.24748
O	9.53126	3.87715	6.65008
O	11.21191	2.78406	4.84582
O	5.15041	1.14000	1.61052
O	7.00845	4.35111	2.73878
O	9.59303	4.23388	2.31027
O	4.37508	2.95186	8.23919
O	10.43241	8.58192	1.05373
O	11.53526	5.58355	1.05622
O	12.56375	12.89669	34.88028
Si	8.77079	5.13575	7.33970
Si	2.01065	5.92876	4.81774
Si	3.96788	1.78196	7.17673
Si	10.17891	8.36801	2.65723
Si	7.41885	9.79404	3.37077
Si	3.31668	10.27934	5.13374
Si	10.72553	5.39091	2.49787
Si	9.72432	2.73145	5.51786
Si	10.24118	12.55748	5.71985
Si	5.12393	11.70071	7.12156
Si	3.40097	9.94044	1.97094
Si	3.50669	6.90821	2.36986
Si	9.59801	8.16081	7.08967
Si	7.91062	10.57965	6.28486
Si	6.11780	5.78683	5.94467
Si	6.37217	7.07386	3.26486
Si	3.79890	7.62147	6.66128
Si	0.48623	9.88290	6.31148
Si	1.31004	1.28845	2.00874
Si	10.71231	12.41628	2.53684
Si	0.80793	11.12700	1.26817
Si	12.00921	8.78159	5.02407
Si	12.45228	3.79686	4.51215
Si	4.25259	2.49753	1.76677
Si	8.29927	3.36595	2.83598
Si	4.02173	3.65013	4.72700
Ta	9.58452	6.76537	9.60730

E= -847,094813 eV

TS(25-25´)

H	4.16510	10.10530	8.43651
H	2.48241	8.58301	8.19196
H	0.02708	9.09569	8.38420
H	1.08985	2.22995	6.41320
H	5.28129	3.29849	8.24176
H	6.34818	10.80501	1.68097
H	8.91014	11.26752	1.66590
H	4.22953	4.42421	0.66194
H	2.33946	5.97605	0.65745
H	8.74725	1.54555	1.72393
H	7.37095	5.90944	1.75008
H	10.97876	1.58110	1.30639
H	12.40202	4.09878	0.80663
H	6.13730	1.29421	1.64373
H	6.10294	3.98610	2.91245
H	10.42782	9.52557	0.80514
H	11.25867	6.33961	0.51254
H	0.30804	12.01068	34.25346
H	4.53052	11.83540	1.40368
H	2.26593	0.64899	8.20440
H	7.98475	7.23438	8.95230
H	12.33550	6.84410	8.91908
H	0.60568	2.88730	9.32162
H	11.87781	4.47602	8.14760
H	11.54614	3.97522	9.82076
H	12.10950	7.44118	11.27661
H	11.81052	5.69376	11.71348
H	9.85357	7.85763	12.17327
H	9.41920	6.10644	12.30912
C	11.89228	6.09775	9.58381
C	12.13472	4.66553	9.19771
C	9.64363	6.93426	11.62702
C	11.76940	6.46398	10.94582
O	4.43791	11.34064	5.67148
O	7.25768	10.78331	2.09588
O	9.90844	11.32509	1.62923
O	4.67034	3.55154	0.60718
O	1.86198	10.62206	5.82101
O	3.19359	5.88420	1.12075

O	5.05638	13.31484	7.28417
O	10.23862	12.37308	4.09555
O	8.56280	2.89244	4.37360
O	2.60583	4.44416	4.54649
O	5.14470	4.59627	5.42842
O	4.61450	10.86473	1.32250
O	10.04400	6.77959	2.91537
O	7.93001	2.09315	1.86562
O	6.22257	8.68163	3.43530
O	3.17312	10.37097	3.52453
O	3.79694	8.38859	1.80563
O	2.70155	6.52373	6.17400
O	2.31133	6.85355	3.48635
O	3.83144	8.79283	5.53596
O	7.17947	5.08185	6.98437
O	8.86461	9.06237	3.28341
O	10.13683	8.35088	8.66536
O	10.82197	8.63706	6.10544
O	8.28602	9.07053	6.77781
O	7.40818	10.64307	4.75635
O	2.00343	10.04031	1.11919
O	7.29389	6.86077	1.94324
O	9.30392	11.45190	6.44312
O	6.92243	6.47299	4.70782
O	9.63062	1.25419	6.17119
O	9.41782	6.56207	6.81968
O	4.88445	6.38313	3.07222
O	5.26548	6.90555	6.76951
O	9.05571	5.03559	8.96974
O	6.69876	11.20992	7.18547
O	2.40901	1.30270	7.50438
O	4.27304	11.07254	8.37007
O	3.41908	8.25862	8.12726
O	0.26476	8.58823	5.36973
O	11.84110	5.01333	3.61693
O	0.39985	5.95431	5.06849
O	1.59954	12.45996	1.75754
O	11.79246	12.39678	6.27133
O	12.32100	12.13151	2.36865
O	0.79562	9.42417	7.87752
O	11.45729	8.95465	3.50456
O	10.39524	13.93739	1.99292
O	0.50857	2.81496	5.88043
O	0.09671	1.64141	0.96301
O	0.94062	1.47878	3.57890
O	3.85071	2.32904	5.64416
O	2.67387	2.11274	1.67560
O	4.56504	3.19142	3.24994
O	9.53806	3.88881	6.63138
O	11.21402	2.78334	4.83565
O	5.15375	1.13904	1.61082
O	7.00968	4.34869	2.73602
O	9.59483	4.23324	2.30865
O	4.36654	2.95347	8.23937
O	10.43112	8.58300	1.05231
O	11.53606	5.58179	1.05228
O	12.56698	12.89357	34.88161
Si	8.77950	5.13593	7.34197
Si	2.01680	5.92946	4.81830
Si	3.96688	1.78147	7.17843
Si	10.18155	8.36747	2.65607
Si	7.42250	9.78875	3.38254
Si	3.32425	10.27929	5.13655
Si	10.72766	5.39017	2.49466
Si	9.72705	2.73288	5.50867
Si	10.24677	12.56254	5.72066
Si	5.12771	11.70259	7.12524
Si	3.40494	9.93909	1.97326
Si	3.51329	6.90752	2.37288
Si	9.61640	8.17050	7.09901
Si	7.91866	10.58480	6.29955
Si	6.12323	5.78002	5.95676
Si	6.37670	7.06764	3.27601
Si	3.80383	7.62089	6.66470
Si	0.49127	9.88462	6.30969
Si	1.31451	1.28780	2.00613
Si	10.71407	12.41704	2.53792
Si	0.81110	11.12561	1.26930
Si	12.01663	8.78346	5.01847
Si	12.45531	3.79648	4.50696
Si	4.25706	2.49717	1.76795
Si	8.30045	3.36358	2.83000
Si	4.02720	3.64802	4.73028
Ta	9.59842	6.76039	9.64404

E= -846,728277 eV

25´

H	4.19566	10.11397	8.44735
H	2.51241	8.57860	8.19956
H	0.04719	9.08775	8.38960
H	1.10175	2.20866	6.39328
H	5.26151	3.29536	8.27305
H	6.37533	10.80038	1.67751
H	8.94310	11.25797	1.67515
H	4.26626	4.42073	0.66554
H	2.38896	5.98310	0.64655
H	8.76742	1.54584	1.74834
H	7.38744	5.91915	1.75619
H	10.98874	1.56203	1.27970
H	12.42024	4.09452	0.79517
H	6.15617	1.28272	1.66035
H	6.11848	3.99676	2.91402
H	10.45384	9.53440	0.83047
H	11.24207	6.32090	0.49070
H	0.34343	11.93716	34.22176
H	4.55256	11.83808	1.42182
H	2.30557	0.55008	8.13843
H	7.84520	7.26778	9.15553
H	12.38157	6.62865	8.58924
H	0.80840	2.76234	9.00594
H	11.78291	4.18732	8.31995
H	12.02133	3.93204	10.07641
H	12.08153	7.59837	10.83222
H	11.94473	5.91696	11.57125

H	9.25974	7.97252	12.16952
H	8.76017	6.23040	12.26172
C	12.19986	5.97543	9.44760
C	12.34452	4.51838	9.20624
C	9.13365	7.03676	11.61551
C	12.01506	6.52742	10.67218
O	4.46941	11.33686	5.67139
O	7.28404	10.77430	2.09417
O	9.94219	11.30957	1.65107
O	4.70323	3.54613	0.61145
O	1.89599	10.61488	5.83591
O	3.23200	5.88245	1.12723
O	5.08092	13.31814	7.27692
O	10.26543	12.39653	4.10144
O	8.56599	2.91022	4.40254
O	2.63044	4.44530	4.54082
O	5.16825	4.58977	5.43216
O	4.63655	10.86783	1.33316
O	10.06236	6.77284	2.91615
O	7.94588	2.08653	1.89906
O	6.24028	8.68399	3.45362
O	3.19433	10.36298	3.53365
O	3.83024	8.38776	1.80993
O	2.73114	6.52081	6.17378
O	2.33525	6.85743	3.48668
O	3.86732	8.78714	5.54286
O	7.20273	5.06220	6.98991
O	8.87876	9.05181	3.29707
O	10.09957	8.33424	8.69187
O	10.87591	8.63118	6.15272
O	8.31872	9.08494	6.77148
O	7.43571	10.65796	4.75472
O	2.02749	10.03141	1.12975
O	7.31080	6.86989	1.95209
O	9.33403	11.46569	6.44243
O	6.94913	6.46957	4.71866
O	9.66941	1.26932	6.18494
O	9.39016	6.58209	6.82120
O	4.90786	6.38325	3.09041
O	5.29397	6.89551	6.77959
O	9.07387	5.06125	8.97666
O	6.72856	11.21812	7.18673
O	2.42554	1.26677	7.49861
O	4.29876	11.08077	8.36935
O	3.44857	8.25536	8.13137
O	0.29012	8.59210	5.37158
O	11.87909	5.01845	3.59523
O	0.42889	5.95436	5.07628
O	1.63281	12.45932	1.73796
O	11.82649	12.40516	6.27428
O	12.35047	12.14404	2.38343
O	0.81542	9.41849	7.88438
O	11.46479	8.94859	3.53080
O	10.40943	13.92863	1.97532
O	0.52896	2.80669	5.86667
O	0.12267	1.63957	0.94840
O	0.95519	1.46366	3.56681
O	3.85890	2.32908	5.64660
O	2.69612	2.11751	1.67558
O	4.59071	3.18642	3.25458
O	9.58319	3.90388	6.64512
O	11.22161	2.79758	4.81563
O	5.17239	1.13170	1.61678
O	7.02728	4.35671	2.74181
O	9.61435	4.22455	2.32639
O	4.34987	2.94275	8.24736
O	10.45607	8.58926	1.06918
O	11.53220	5.57095	1.03442
O	12.58211	12.87061	34.88857
Si	8.80207	5.14057	7.35021
Si	2.04462	5.93077	4.81694
Si	3.97717	1.77179	7.17717
Si	10.19778	8.36229	2.66882
Si	7.44171	9.78941	3.38906
Si	3.35559	10.27201	5.14473
Si	10.74608	5.38582	2.48815
Si	9.74913	2.74622	5.51763
Si	10.28038	12.57774	5.72685
Si	5.15688	11.70525	7.12460
Si	3.43098	9.93648	1.98202
Si	3.54346	6.90834	2.37871
Si	9.63814	8.17730	7.10886
Si	7.94851	10.59899	6.29763
Si	6.14945	5.76972	5.96439
Si	6.39984	7.07015	3.29076
Si	3.83375	7.61491	6.67112
Si	0.51923	9.88437	6.31752
Si	1.33769	1.28509	1.99321
Si	10.74083	12.41970	2.54378
Si	0.83775	11.12041	1.27222
Si	12.04455	8.78260	5.03562
Si	12.47562	3.79597	4.48915
Si	4.28124	2.49410	1.77154
Si	8.31320	3.36673	2.85047
Si	4.04859	3.64568	4.73249
Ta	9.47243	6.80054	9.70945

E= -846,853854 eV

26

H	4.11679	10.09270	8.42912
H	2.45536	8.57821	8.20828
H	0.02085	9.04804	8.37440
H	0.97128	2.38223	6.62380
H	5.27115	3.23751	8.31723
H	6.34446	10.80145	1.64472
H	8.92103	11.18267	1.65861
H	4.19847	4.42946	0.68571
H	2.18538	5.83174	0.78034
H	8.74462	1.51610	1.75630
H	7.34142	5.91316	1.78170
H	10.84600	13.97530	1.12313
H	12.47035	4.14335	0.94090
H	6.20020	1.33980	1.66020
H	6.13434	3.99079	2.97859

H	10.41142	9.45714	0.80066
H	11.29678	6.33702	0.60423
H	0.12333	12.71230	34.90053
H	4.52959	11.81788	1.37728
H	2.19331	0.79994	8.32293
H	11.40380	6.33535	10.36307
H	8.91103	8.10321	11.90881
H	8.46148	6.34524	12.05695
C	8.99007	7.10717	11.46629
O	4.39963	11.35733	5.66150
O	7.24684	10.79390	2.07544
O	9.92153	11.19838	1.68883
O	4.66912	3.57202	0.64037
O	1.83533	10.61339	5.81422
O	3.09536	5.86162	1.13463
O	4.99329	13.31929	7.30128
O	10.18027	12.35870	4.13516
O	8.62279	2.86725	4.37266
O	2.57684	4.45397	4.55604
O	5.10441	4.61413	5.45629
O	4.60203	10.84606	1.31572
O	9.93222	6.76369	2.94102
O	7.94020	2.09293	1.87766
O	6.15836	8.71844	3.39958
O	3.15517	10.34730	3.51968
O	3.64358	8.39678	1.74130
O	2.68984	6.53655	6.17681
O	2.24746	6.86360	3.49431
O	3.82548	8.80143	5.54779
O	7.16519	5.10651	6.96787
O	8.80693	9.05723	3.31119
O	9.94869	8.28166	8.64320
O	10.81948	8.68748	6.13795
O	8.22780	9.07268	6.74320
O	7.36269	10.67095	4.74426
O	1.95754	10.21871	1.11136
O	7.23090	6.86827	1.93838
O	9.24731	11.45557	6.47331
O	6.84113	6.51102	4.69659
O	9.63430	1.25639	6.21290
O	9.33297	6.59509	6.70146
O	4.81257	6.43186	3.04203
O	5.24825	6.91945	6.80447
O	9.03328	5.17298	8.91541
O	6.64119	11.21316	7.18370
O	2.34878	1.34110	7.53324
O	4.21998	11.06096	8.36370
O	3.39813	8.26994	8.14012
O	0.24018	8.60222	5.31540
O	11.72665	5.08625	3.78840
O	0.37288	5.96139	5.09789
O	1.53237	12.51286	2.16497
O	11.75989	12.36514	6.29842
O	12.29321	12.08110	2.45089
O	0.78302	9.36289	7.85084
O	11.40047	8.91226	3.50877
O	10.33700	13.81549	1.95037
O	0.37097	2.94604	6.08716
O	0.16680	1.69033	1.11906
O	1.02634	1.75506	3.75887
O	3.80483	2.34086	5.66623
O	2.73147	2.08417	1.75313
O	4.59000	3.21711	3.29059
O	9.53446	3.89782	6.63645
O	11.27015	2.77818	4.90584
O	5.21686	1.17352	1.64170
O	7.04037	4.34959	2.78496
O	9.62222	4.21466	2.30418
O	4.33433	2.96506	8.25822
O	10.36124	8.52024	1.06150
O	11.60670	5.62642	1.19100
O	12.54278	13.31479	0.11888
Si	8.77258	5.16649	7.28376
Si	1.98857	5.93969	4.83291
Si	3.91315	1.79645	7.20312
Si	10.10790	8.34492	2.66915
Si	7.37578	9.80894	3.37371
Si	3.30067	10.27891	5.13177
Si	10.70092	5.40446	2.57352
Si	9.75963	2.72378	5.53316
Si	10.21479	12.55151	5.76047
Si	5.06759	11.70911	7.12826
Si	3.34939	9.96515	1.95130
Si	3.42254	6.92108	2.35297
Si	9.56675	8.17631	7.03071
Si	7.85878	10.60159	6.29183
Si	6.08379	5.80109	5.95950
Si	6.30615	7.10126	3.25945
Si	3.78464	7.63402	6.68072
Si	0.47053	9.86658	6.30054
Si	1.35101	1.37276	2.21590
Si	10.67634	12.33307	2.58751
Si	0.77055	11.26920	1.45017
Si	11.99411	8.78818	5.01196
Si	12.43078	3.91414	4.67081
Si	4.30097	2.51247	1.80998
Si	8.32699	3.35621	2.84054
Si	3.99817	3.65734	4.75446
Ta	9.78444	6.72938	9.74714

E= -798,053016eV

XII. Comparison between PBE0 and M06 functionals

XII1. PBE0

Hydrogen molecule

H	0.000000	0.000000	0.373179

H	0.000000	0.000000	-0.373179

E_{SCF}= -1,168158 au
E_{disp}= -0,0433 kcal·mol^{-1}

Ethane

C	0.000000	0.000000	0.760870
H	-0.509031	0.882221	1.159898
H	1.018541	-0.000277	1.159898
H	-0.509510	-0.881944	1.159898
C	0.000000	0.000000	-0.760870
H	0.509510	-0.881944	-1.159898
H	-1.018541	-0.000277	-1.159898
H	0.509031	0.882221	-1.159898

E_{SCF}= -79,743240 au
E_{disp}= -1,6652 kcal·mol^{-1}

Ethene

C	0.663325	0.000000	0.000004
C	-0.663325	0.000000	-0.000003
H	1.233575	0.924134	-0.000010
H	1.233575	-0.924134	0.000023
H	-1.233575	-0.924134	0.000010
H	-1.233575	0.924134	-0.000023

E_{SCF}= -78,504342 au
E_{disp}= -1,1934 kcal·mol^{-1}

1a (singlet)

Ta	-1.470918	-0.000090	-0.000066
O	-0.366688	-1.485908	-0.021957
O	-0.366890	1.485882	0.021743
Si	1.294276	-1.540049	-0.002828
Si	1.294068	1.540213	0.002701
O	1.853146	0.000120	-0.000571
O	1.885634	-2.228892	-1.359152
H	1.666778	-3.143772	-1.538061
O	1.690549	-2.350176	1.356549
H	2.603012	-2.347617	1.646316
O	1.885249	2.228268	1.359507
H	1.665894	3.142867	1.539247
O	1.690359	2.351206	-1.356145
H	2.602788	2.348658	-1.646016
H	-3.258137	-0.000226	0.000438

E_{SCF}= -1166,179053 au
E_{disp}= -9,7174 kcal·mol^{-1}

TS(1a-1b)

Ta	1.361065	-0.097581	0.026315
O	0.574823	1.597287	-0.206584
O	0.328651	-1.667244	-0.120980
Si	-1.074220	1.647684	-0.008265
Si	-1.315258	-1.474791	-0.000663
O	-1.664683	0.121840	-0.198467
O	-1.782558	2.511955	-1.199805
H	-1.564882	3.441470	-1.273638
O	-1.347831	2.255855	1.482145
H	-2.216774	2.154937	1.871231
O	-1.897693	-1.883351	1.471446
H	-1.734725	-2.767430	1.801272
O	-1.950784	-2.360593	-1.215740
H	-2.895528	-2.320653	-1.366081
H	0.548011	-0.098075	-2.160409
H	1.328602	-0.154280	-2.102298
H	2.550856	-0.159093	1.337765

E_{SCF}= -1167,332346 au
E_{disp}= -11,2810 kcal·mol^{-1}

1b

Ta	1.440180	-0.000007	0.000002
O	0.345638	-1.518406	0.027124
O	0.345656	1.518403	-0.027125
Si	-1.314333	-1.553750	0.003571
Si	-1.314316	1.553764	-0.003582
O	-1.838536	0.000010	-0.000036
O	-1.922880	-2.225486	1.360031
H	-1.709652	-3.138655	1.554552
O	-1.717904	-2.346793	-1.362451
H	-2.637064	-2.380466	-1.628305
O	-1.922840	2.225558	-1.360022
H	-1.709644	3.138748	-1.554477
O	-1.717887	2.346762	1.362467
H	-2.637032	2.380325	1.628384
H	3.188833	-0.000014	0.000013
H	2.180918	0.020258	1.581436
H	2.180939	-0.020287	-1.581422

E_{SCF}= -1167,418848 au
E_{disp}= -10,7731 kcal·mol^{-1}

TS(1a-3a)

Ta	1.037274	-0.016356	-0.352773
O	-0.067453	1.491013	-0.170897
O	-0.088288	-1.498280	-0.110700
Si	-1.684113	1.550860	0.160161
Si	-1.715405	-1.528143	0.174381
O	-2.244797	0.017472	0.312914
O	-2.539634	2.212514	-1.067034
H	-2.297792	3.089596	-1.365149
O	-1.825793	2.392310	1.555609
H	-2.693478	2.464859	1.953820
O	-2.063966	-2.246562	1.602596
H	-1.915528	-3.189545	1.675842
O	-2.393292	-2.302700	-1.095953
H	-3.334709	-2.203464	-1.238502
C	3.119562	0.008543	0.935456
H	2.857899	0.904478	1.503847
H	2.862727	-0.852743	1.556618
C	4.626317	0.003272	0.621646
H	5.208545	0.034112	1.546726
H	4.914918	-0.896073	0.069272
H	4.909515	0.868147	0.014162
H	2.033827	-0.047752	-1.806298
H	2.845133	-0.026568	-0.301405

E_{SCF}= -1245,914010 au
E_{disp}= -13,9197 kcal·mol^{-1}

TS(1b-2)

Ta	-1.082731	-0.386093	-0.398410
O	-0.169156	1.293513	-0.247712
O	0.425762	-1.477473	-0.053312
Si	1.384815	1.745300	0.012605
Si	2.007362	-1.217180	0.313124
O	2.285942	0.394988	0.255699
O	1.544013	2.626676	1.385889
H	1.178415	3.511544	1.389953
O	1.870477	2.569693	-1.314976
H	2.809053	2.708182	-1.443021
O	3.013386	-1.889800	-0.786248
H	2.993221	-2.840884	-0.894330
O	2.223848	-1.816802	1.821867
H	3.053268	-1.635705	2.264776
C	-2.769228	0.698380	0.745984
C	-4.203907	0.316015	1.084522
H	-4.669522	-0.217664	0.252289
H	-4.249832	-0.337256	1.962897
H	-4.810285	1.199299	1.308167
H	-1.065509	-0.427683	-2.134269
H	-2.587671	-1.009620	-1.106166
H	-1.908978	-1.592786	0.805304
H	-2.766038	1.359984	-0.139414
H	-2.298016	1.261474	1.559324
H	-2.349845	-0.749274	0.895573

E_{SCF}= -1247,126348 au

E_{disp}= -15,8189 kcal·mol^{-1}

2

Ta	1.114687	-0.212096	-0.457815
O	-0.231132	-1.461121	-0.064147
O	0.077431	1.390767	-0.237332
Si	-1.850385	-1.369768	0.259001
Si	-1.495170	1.661070	0.126908
O	-2.238433	0.213360	0.366322
O	-2.206416	-2.028694	1.712098
H	-2.152615	-2.980624	1.799915
O	-2.603585	-2.124288	-0.979739
H	-3.539469	-1.970283	-1.110259
O	-2.321467	2.361827	-1.101511
H	-1.985216	3.186147	-1.453947
O	-1.501480	2.562451	1.493254
H	-2.346150	2.769746	1.893552
C	2.455239	-0.128749	1.211423
H	1.854258	0.356930	1.999386
H	2.374981	-1.215648	1.423975
C	3.910573	0.300811	1.292946
H	4.503445	-0.180885	0.510935
H	4.009589	1.383910	1.166349
H	1.157408	0.116866	-2.180590
H	2.499680	-1.051730	-1.222860
H	2.342261	1.164711	-1.447895
H	2.680119	1.193669	-0.743229
H	4.361972	0.048583	2.259153

E_{SCF}= -1247,149684 au

E_{disp}= -15,8608 kcal·mol^{-1}

3a

Ta	1.082822	-0.379289	-0.434157
O	-0.314165	-1.558417	-0.018391
O	0.329479	1.354109	-0.332018
Si	-1.907696	-1.225738	0.301705
Si	-1.223124	1.776286	0.027140
O	-2.079902	0.400705	0.300991
O	-2.331400	-1.723754	1.798242
H	-2.352929	-2.664391	1.976137
O	-2.761257	-1.950192	-0.885847
H	-3.686012	-1.727147	-0.994566
O	-1.971776	2.510747	-1.225858
H	-1.559775	3.285464	-1.609453
O	-1.135804	2.704232	1.368610
H	-1.949620	3.001003	1.776391
C	2.427388	-0.188979	1.224899
H	1.800268	0.236469	2.029113
H	2.669325	-1.216639	1.537021
C	3.703349	0.629203	1.059947
H	4.261222	0.711263	2.000019
H	4.363764	0.175142	0.316492
H	3.486319	1.650578	0.728909
H	1.274582	-0.240917	-2.170163
H	2.608859	-1.067187	-0.987493

E_{SCF}= -1245,976026 au

E_{disp}= -14,6723 kcal·mol^{-1}

3b

Ta	1.175540	-0.415244	-0.238997
O	-0.350419	-1.471782	0.013237
O	0.288634	1.288629	-0.134922
Si	-1.977024	-1.207790	0.157690
Si	-1.273138	1.753608	0.009264
O	-2.203303	0.408733	0.192949
O	-2.551662	-1.787144	1.573846
H	-2.608055	-2.736737	1.682569
O	-2.668874	-1.916423	-1.142525
H	-3.562140	-1.666532	-1.379685
O	-1.852306	2.485361	-1.337273
H	-1.363150	3.230626	-1.686671
O	-1.349153	2.711924	1.334243
H	-2.206048	3.044801	1.601743
C	2.590411	-0.030106	1.295256
H	2.199845	0.526343	2.148573
H	3.135183	-0.914665	1.627683
C	3.347117	0.812671	0.290804
H	3.350136	1.874929	0.537528
H	4.358999	0.456718	0.099397
H	2.888320	0.784675	-0.755400
H	1.495634	0.019676	-1.896934
H	2.435168	-1.528521	-0.882890

E_{SCF}= -1245,980387 au

E_{disp}= -14,9303 kcal·mol^{-1}

TS(3b-4)

Ta	-1.178560	-0.409508	-0.328610

O	-0.228616	1.262298	-0.229724
O	0.312039	-1.504971	0.011964
Si	1.320532	1.734311	-0.005318
Si	1.919183	-1.253327	0.260586
O	2.205338	0.355737	0.191752
O	1.361613	2.681168	1.324964
H	2.085674	3.302216	1.404697
O	1.942105	2.609557	-1.240635
H	2.221723	2.148558	-2.031956
O	2.828707	-1.916203	-0.928404
H	2.755110	-2.859436	-1.076442
O	2.251136	-1.875884	1.737227
H	3.135326	-1.765258	2.087339
C	-2.865001	1.245549	0.629181
H	-2.208660	2.006274	1.032833
H	-3.349874	1.452911	-0.322009
C	-3.222054	0.161098	1.359022
H	-2.862796	0.028406	2.374846
H	-4.000078	-0.516178	1.032025
H	-2.060050	-1.381570	0.875099
H	-1.061445	-0.678038	-2.043087
H	-2.721932	-0.900528	-1.050333

E_{SCF}= -1245,927550 au

E_{disp}= -15,0213 kcal·mol^{-1}

4

Ta	1.081861	-0.635792	-0.006981
O	0.457183	1.176614	0.000763
O	-0.575304	-1.503343	-0.019837
Si	-1.024494	1.882275	-0.011636
Si	-2.147290	-0.982747	-0.003364
O	-2.126039	0.650655	0.015525
O	-1.138392	2.778908	-1.366745
H	-1.738027	3.524919	-1.361101
O	-1.297363	2.864431	1.268032
H	-1.592003	2.473640	2.090965
O	-2.911542	-1.434614	1.370017
H	-3.032979	-2.370095	1.535441
O	-2.831580	-1.594262	-1.353578
H	-3.714849	-1.313434	-1.593190
C	3.334682	0.712885	0.716439
H	2.818137	1.503277	1.250399
H	3.911677	0.011305	1.306050
C	3.375190	0.694004	-0.630603
H	2.891959	1.467959	-1.217866
H	3.986201	-0.022814	-1.164904
H	1.820630	-0.712504	-1.594985
H	1.712830	-0.669810	1.627090
H	2.418372	-1.819227	0.067514

E_{SCF}= -1245,936847 au

E_{disp}= -15,1121 kcal·mol^{-1}

TS(3a-5)

Ta	1.232289	-0.232049	-0.248360
O	-0.196004	-1.451651	-0.005896
O	0.091110	1.303899	-0.056244
Si	-1.830536	-1.394098	0.165580
Si	-1.499676	1.614939	0.120768
O	-2.277745	0.174923	0.273677
O	-2.319020	-2.110362	1.554216
H	-2.253353	-3.063798	1.609680
O	-2.459698	-2.122320	-1.160892
H	-3.385611	-1.976721	-1.356603
O	-2.175100	2.329437	-1.192818
H	-1.820615	3.173792	-1.472082
O	-1.662132	2.530210	1.470154
H	-2.549072	2.741398	1.762205
C	2.704068	-0.410397	1.031261
H	2.923519	-1.052479	1.882555
H	2.692133	-1.403697	-0.280052
C	3.671170	0.731761	0.786165
H	4.671408	0.387006	0.502956
H	3.343521	1.397986	-0.029930
H	3.756745	1.345192	1.688886
H	1.905351	0.420671	-1.754312
H	2.128027	-1.659268	-1.092561

E_{SCF}= -1245,939227 au

E_{disp}= -14,7910 kcal·mol^{-1}

5

Ta	1.214292	-0.284489	-0.265584
O	-0.254948	-1.462119	-0.003342
O	0.177937	1.317549	-0.192150
Si	-1.877496	-1.294823	0.198920
Si	-1.396338	1.698658	0.023116
O	-2.235937	0.301101	0.222340
O	-2.384292	-1.896191	1.634796
H	-2.336320	-2.843443	1.764378
O	-2.571701	-2.058641	-1.074438
H	-3.501751	-1.902000	-1.239634
O	-2.059812	2.420993	-1.290614
H	-1.705801	3.268693	-1.560103
O	-1.481506	2.644360	1.357973
H	-2.349160	2.849634	1.706801
C	2.530209	-0.289607	1.135060
H	2.701639	-0.747818	2.106613
H	2.417936	-1.931911	-0.505985
C	3.397140	0.899872	0.773005
H	4.442481	0.625285	0.595308
H	3.073943	1.386425	-0.169511
H	3.358362	1.669355	1.552837
H	2.058553	0.050382	-1.798534
H	1.889588	-2.071136	-1.085790

E_{SCF}= -1245,944399 au

E_{disp}= -14,8962 kcal·mol^{-1}

6

Ta	1.119821	-0.091402	-0.411732
O	0.095218	1.479970	-0.246851
O	-0.067656	-1.531517	-0.042764
Si	-1.512380	1.630169	0.117412
Si	-1.689491	-1.456913	0.232824
O	-2.139043	0.123370	0.246162
O	-2.340474	2.356438	-1.089293
H	-2.122985	3.263307	-1.306343

O	-1.576753	2.452012	1.528246
H	-2.413502	2.503732	1.990789
O	-2.090797	-2.030863	1.711630
H	-1.849484	-2.932933	1.923664
O	-2.401941	-2.278150	-0.987286
H	-3.358098	-2.290163	-1.034544
C	2.765967	-0.216434	0.519990
C	3.901676	0.296103	1.337621
H	2.743257	-1.334704	0.411204
H	4.864809	0.052857	0.873585
H	3.851360	1.383710	1.436090
H	1.760762	-0.286906	-2.040977
H	3.909986	-0.128795	2.348406

E_{SCF}= -1244,775073 au

E_{disp}= -13,2253 kcal·mol^{-1}

XII2. M06

Hydrogen molecule

H	0.00000	0.00000	0.37308
H	0.00000	0.00000	-0.37308

E_{SCF}= -1,170395 au

Ethane

C	0.00000	0.00000	0.75855
H	-0.50845	0.88212	1.16004
H	1.01816	-0.00073	1.16004
H	-0.50971	-0.88139	1.16004
C	0.00000	0.00000	-0.75855
H	0.50971	-0.88139	-1.16004
H	-1.01816	-0.00073	-1.16004
H	0.50845	0.88212	-1.16004

E_{SCF}= -79,776211au

Ethene

C	0.66140	0.00000	0.00000
C	-0.66140	0.00000	0.00000
H	1.23349	0.92328	-0.00001
H	1.23349	-0.92328	0.00002
H	-1.23349	-0.92328	0.00001
H	-1.23349	0.92328	-0.00002

E_{SCF}= -78,538546 au

1a (singlet)

Ta	-1.46687	-0.00005	-0.00002
O	-0.36924	1.49562	0.02225
O	-0.36912	-1.49561	-0.02292
Si	1.28662	1.54033	-0.00022
Si	1.28674	-1.54023	0.00005
O	1.83131	0.00007	-0.00078
O	1.87189	2.22518	1.35323
H	1.66715	3.13990	1.54500
O	1.69595	2.33664	-1.35664
H	2.57163	2.22889	-1.72625
O	1.87249	-2.22639	-1.35251
H	1.66829	-3.14147	-1.54313
O	1.69562	-2.33524	1.35738
H	2.57121	-2.22724	1.72713
H	-3.25501	-0.00015	0.00103

E_{SCF}= -1166,693132 au

TS(1a-1b)

Ta	1.36226	-0.08514	0.02297
O	0.55703	1.61181	-0.16356
O	0.33978	-1.67102	-0.04221
Si	-1.08928	1.64725	-0.00071
Si	-1.30314	-1.49449	0.00727
O	-1.63771	0.10579	-0.12506
O	-1.79030	2.44352	-1.23481
H	-1.56955	3.36282	-1.38220
O	-1.39893	2.29573	1.45859
H	-2.26919	2.20379	1.84537
O	-1.93890	-1.96786	1.42926
H	-1.77491	-2.85480	1.74886
O	-1.87681	-2.31476	-1.27457
H	-2.80381	-2.25223	-1.50289
H	0.50162	-0.10428	-2.08333
H	1.30350	-0.17136	-2.04260
H	2.62783	-0.13274	1.26693

E_{SCF}= -1167,849474 au

1b

Ta	1.43805	-0.00001	0.00000
O	0.34571	-1.52193	0.02404
O	0.34574	1.52193	-0.02403
Si	-1.30959	-1.55221	0.00188
Si	-1.30957	1.55222	-0.00191
O	-1.82173	0.00001	-0.00015
O	-1.91259	-2.22062	1.35521
H	-1.69743	-3.12777	1.57098
O	-1.72043	-2.33747	-1.35901
H	-2.63112	-2.35180	-1.65159
O	-1.91254	2.22086	-1.35515
H	-1.69726	3.12800	-1.57083
O	-1.72042	2.33726	1.35909
H	-2.63113	2.35163	1.65162
H	3.19208	-0.00002	0.00000
H	2.16254	0.01671	1.59402
H	2.16253	-0.01674	-1.59402

E_{SCF}= -1167,927537au

TS(1a-3a)

Ta	1.02513	-0.01656	-0.32105
O	-0.02350	1.52925	-0.10636
O	-0.08845	-1.49603	-0.02421
Si	-1.65176	1.57418	0.15260
Si	-1.73316	-1.52112	0.17493
O	-2.18009	0.04161	0.33953
O	-2.44685	2.16653	-1.14158
H	-2.21939	3.03600	-1.46991
O	-1.87479	2.45927	1.50091
H	-2.74939	2.50822	1.88599
O	-2.18115	-2.31327	1.51737
H	-2.42468	-3.23518	1.43808

O	-2.43395	-2.26602	-1.09345
H	-2.15233	-2.03662	-1.97988
C	3.12162	-0.02074	0.90355
H	2.88927	0.88391	1.47487
H	2.86240	-0.87512	1.53684
C	4.61780	-0.05468	0.56466
H	5.22215	-0.03257	1.47628
H	4.87965	-0.96036	0.00761
H	4.90567	0.80315	-0.05210
H	1.89830	-0.08346	-1.85688
H	2.83618	-0.06011	-0.35689

E_{SCF}= -1246,455857 au

TS(1b-2)

Ta	-1.06878	-0.42606	-0.36527
O	-0.19124	1.27899	-0.24348
O	0.46182	-1.47476	-0.00207
Si	1.35228	1.76224	-0.00812
Si	2.04623	-1.17828	0.30531
O	2.28031	0.43325	0.21428
O	1.51143	2.63856	1.36184
H	1.13174	3.51623	1.38960
O	1.80045	2.59927	-1.33344
H	2.73042	2.75525	-1.49419
O	3.02186	-1.84247	-0.81752
H	3.02316	-2.79257	-0.92943
O	2.32946	-1.75079	1.80657
H	3.16528	-1.55352	2.22847
C	-2.81658	0.72134	0.70148
C	-4.25511	0.34236	1.00384
H	-4.66526	-0.28461	0.20650
H	-4.33199	-0.22470	1.93876
H	-4.89459	1.22490	1.10807
H	-1.00295	-0.53924	-2.10141
H	-2.56814	-1.09627	-1.05901
H	-1.90539	-1.53126	0.91889
H	-2.77438	1.28431	-0.25041
H	-2.38271	1.36733	1.47285
H	-2.36620	-0.63724	0.95431

E_{SCF}= -1247,669364 au

2

Ta	1.10566	-0.20665	-0.44611
O	-0.22061	-1.46427	-0.05411
O	0.07377	1.40437	-0.22771
Si	-1.84300	-1.37282	0.25039
Si	-1.49813	1.66065	0.12786
O	-2.22892	0.20570	0.32934
O	-2.19732	-2.01691	1.70271
H	-2.16751	-2.96720	1.80976
O	-2.58394	-2.14133	-0.97799
H	-3.48946	-1.92328	-1.19615
O	-2.31587	2.37760	-1.08871
H	-1.99344	3.21083	-1.43100
O	-1.52470	2.52961	1.50775
H	-2.36699	2.72261	1.91851
C	2.45415	-0.13011	1.21821
H	1.86367	0.36447	2.01034
H	2.35757	-1.21750	1.42781
C	3.91189	0.27809	1.27297
H	4.48095	-0.20171	0.47030
H	4.02374	1.36189	1.15414
H	1.12056	0.07490	-2.18236
H	2.50636	-1.05401	-1.18242
H	2.39847	1.28030	-1.46121
H	2.72489	1.34578	-0.76876
H	4.38839	0.01243	2.22433

E_{SCF}= -1247,696904 au

3a

Ta	1.05982	-0.47974	-0.49443
O	-0.39337	-1.60746	-0.10619
O	0.44540	1.29634	-0.61874
Si	-1.89579	-1.11045	0.37034
Si	-1.01473	1.83546	-0.07618
O	-1.91117	0.52116	0.30380
O	-2.18117	-1.48652	1.92803
H	-2.18966	-2.40428	2.19889
O	-2.94718	-1.78476	-0.66889
H	-3.86547	-1.51649	-0.66166
O	-1.84576	2.62829	-1.22672
H	-1.47685	3.42446	-1.60857
O	-0.68232	2.73974	1.23566
H	-1.39180	3.03403	1.80616
C	1.97113	-0.20516	1.44346
H	1.11800	0.14350	2.06050
H	2.27562	-1.17879	1.84926
C	3.11382	0.79548	1.51313
H	3.46460	0.95551	2.54020
H	3.96976	0.45409	0.92133
H	2.81159	1.77470	1.12280
H	1.58313	-0.69897	-2.16571
H	2.69622	-1.11343	-0.60293

E_{SCF}= -1246,519515 au

3b

Ta	1.17200	-0.40929	-0.23957
O	-0.35234	-1.45877	0.01958
O	0.28124	1.30053	-0.12517
Si	-1.97731	-1.19955	0.16635
Si	-1.27791	1.75884	0.00214
O	-2.19846	0.41132	0.17723
O	-2.52994	-1.76795	1.58759
H	-2.65312	-2.71047	1.69576
O	-2.68373	-1.92165	-1.11067
H	-3.51319	-1.58248	-1.44532
O	-1.84739	2.47880	-1.34826
H	-1.37837	3.23510	-1.69963
O	-1.37900	2.71600	1.31912
H	-2.23862	3.02573	1.60268
C	2.57834	-0.02492	1.30462
H	2.17692	0.52653	2.15686
H	3.11062	-0.91746	1.63878
C	3.36061	0.82246	0.32481

H	3.36854	1.88115	0.59088
H	4.37683	0.46296	0.15716
H	2.92799	0.81661	-0.72447
H	1.47927	0.02943	-1.90483
H	2.40344	-1.57051	-0.87021

E_{SCF}= -1246,525173 au

TS(3b-4)

Ta	-1.18686	-0.33627	-0.30622
O	-0.15044	1.27402	-0.17430
O	0.20797	-1.50921	0.21764
Si	1.42360	1.64867	0.05589
Si	1.82636	-1.27540	0.31716
O	2.11141	0.28933	0.68625
O	1.51071	2.90328	1.08296
H	2.29145	3.45554	1.05732
O	2.20160	2.05317	-1.32199
H	2.49032	1.33391	-1.88806
O	2.51265	-1.46482	-1.16435
H	2.29606	-2.24288	-1.67865
O	2.40776	-2.28627	1.44704
H	3.32480	-2.21902	1.71088
C	-2.82468	1.26351	0.60203
H	-2.22504	1.94274	1.19815
H	-3.14752	1.61493	-0.37728
C	-3.38683	0.15427	1.15134
H	-3.24078	-0.08813	2.19925
H	-4.14889	-0.41757	0.63569
H	-2.21629	-1.31501	0.81397
H	-0.78337	-0.63744	-1.97843
H	-2.64336	-0.68743	-1.26788

E_{SCF}= -1246,471827 au

4

Ta	1.05652	-0.65205	-0.00844
O	0.46870	1.17608	0.00054
O	-0.59558	-1.51439	-0.02556
Si	-1.00591	1.88655	-0.01071
Si	-2.15757	-0.96731	-0.00334
O	-2.10344	0.65864	0.01418
O	-1.13090	2.78277	-1.35867
H	-1.66262	3.57746	-1.32963
O	-1.27272	2.86612	1.26488
H	-1.55412	2.49110	2.09903
O	-2.91263	-1.40829	1.37057
H	-3.06767	-2.33655	1.54414
O	-2.85537	-1.56368	-1.34522
H	-3.70839	-1.23525	-1.62722
C	3.38514	0.72531	0.71096
H	2.86619	1.50485	1.26014
H	3.93859	-0.00183	1.29459
C	3.41736	0.71737	-0.62738
H	2.92389	1.48874	-1.21118
H	3.99859	-0.01598	-1.17493
H	1.77422	-0.78796	-1.61057
H	1.66231	-0.75080	1.64168
H	2.39270	-1.83782	0.05985

E_{SCF}= -1246,483238 au

TS(3a-5)

Ta	1.21061	-0.19346	-0.28652
O	-0.25497	-1.38216	-0.14843
O	0.08858	1.35167	-0.00985
Si	-1.86481	-1.35857	0.16319
Si	-1.50478	1.65705	0.08586
O	-2.28136	0.22308	0.23192
O	-2.10693	-2.14036	1.56714
H	-2.93698	-2.59997	1.68947
O	-2.76334	-2.11250	-0.97159
H	-3.00053	-1.63750	-1.76771
O	-2.11269	2.32306	-1.28180
H	-1.75461	3.15850	-1.58059
O	-1.74242	2.61043	1.38920
H	-2.63808	2.84404	1.63059
C	2.67121	-0.46578	0.99346
H	2.91797	-1.12095	1.82520
H	2.68077	-1.36180	-0.28710
C	3.57699	0.72620	0.76297
H	4.57975	0.45205	0.41655
H	3.18410	1.41614	-0.00870
H	3.66996	1.30798	1.68579
H	1.87751	0.54218	-1.75819
H	2.11585	-1.60523	-1.16711

E_{SCF}= -1246,484830 au

5

Ta	1.20237	-0.28749	-0.28107
O	-0.26797	-1.46951	-0.01658
O	0.17975	1.32261	-0.23778
Si	-1.88163	-1.28342	0.20419
Si	-1.38865	1.70480	-0.00636
O	-2.22237	0.31127	0.19344
O	-2.36877	-1.84367	1.65655
H	-2.33303	-2.78473	1.82384
O	-2.60477	-2.06465	-1.03432
H	-3.52324	-1.87607	-1.22472
O	-2.05445	2.43169	-1.30856
H	-1.71182	3.28081	-1.58567
O	-1.46142	2.64212	1.32792
H	-2.31733	2.83290	1.71051
C	2.48474	-0.26766	1.14172
H	2.64250	-0.70971	2.12288
H	2.38524	-2.06849	-0.52853
C	3.30696	0.95433	0.79376
H	4.36876	0.72495	0.64648
H	2.99197	1.41992	-0.16218
H	3.21419	1.73352	1.56086
H	2.09956	-0.00970	-1.80086
H	1.84370	-2.21505	-1.07272

E_{SCF}= -1246,493115 au

6

Ta	1.11487	-0.07790	-0.39906
O	0.06361	1.47351	-0.22218

O	-0.02806	-1.55763	-0.02814
Si	-1.55373	1.60580	0.13378
Si	-1.65201	-1.49877	0.21412
O	-2.10625	0.07296	0.17759
O	-2.29336	2.51784	-0.99382
H	-2.09621	2.39122	-1.92129
O	-1.81408	2.28735	1.57995
H	-1.87790	3.23989	1.64132
O	-2.07446	-2.06429	1.68194
H	-1.74022	-2.91460	1.96599
O	-2.33647	-2.32992	-1.00900
H	-3.27925	-2.49198	-0.99164
C	2.77583	-0.16790	0.50781
C	3.90534	0.32192	1.34035
H	2.75833	-1.28337	0.35472
H	4.87280	0.10572	0.87026
H	3.84785	1.40582	1.47658
H	1.71468	-0.25214	-2.05264
H	3.92047	-0.13484	2.33793

E_{SCF}= -1245,319367 au