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Intermolecular Acetaldehyde and Dimethoxymethane Formation Mechanisms via Ethenol and Methoxymethylene Precursors in Reactions of Atomic Carbon with Methanol; A Computational Study

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Details of the Computational Procedure, Applicability of Coupled Clusters Approach, and Benchmarking Details of the Preferred Level of Theory

In inspecting the entrance channel of the C(^{1}D) reaction where the reactants as well as the addition complexes might have significant multi-reference character, originating from the five-fold degeneracy of the ^{1}D state of carbon atom, employing a single determinant approach is questionable. For similar concerns our work on C+H_2O system mainly used MCSCF approaches, however the energy difference of C(^{1}D) + H_2O was off by 3.3 and 4.1 kcal/mol when MCQDPT2 with two different active spaces is employed. On the other hand that error is only 0.8 kcal/mol with the CCSD(T)/cc-pVTZ methodology which is one system where the single reference CCSD(T) formalism is expected to be error prone at first glance. This agreement is mainly due to fortuitous error cancellation among species with similar electronic structure such as initial closed shell species on the OH-insertion path and two important open-shell singlet species on the CH-insertion path. (vide infra) Below MCSCF calculations on selected species as well as a through analysis of electronic states of atomic carbon are presented. The discussion is firstly on the absolute energies of ^{3}P, ^{1}D, and ^{1}S carbon atoms and secondly on the multi-reference calculations regarding the initial phase of C(^{1}D) + CH_3OH reaction.

I. Full CI Benchmarking of Carbon Atom Total Energies

CCSD(T) is a powerful and practical approach whose performance in achieving chemical accuracy is tied to an adequate single reference description of the electronic state of interest. Electronic states that require more than one Hartree-Fock determinant for a qualitatively correct description need special attention. This problem of substantial multireference character is present in the reactions of singlet C(^{1}D) atoms studied in this work. The most difficult part of the singlet PES involves the initial path of attack of the C(^{1}D) atom to the substrate. Indeed, the isolated C(^{1}D) atom with five-fold spatial degeneracy has this problem as none of the five states can be adequately approximated by a single determinant. For a given basis set and a specified electronic spin, exact solutions of the nonrelativistic Schrodinger equation can be obtained by a full CI calculation. Carbon atom is a small system for which full CI calculations with relatively large basis sets are feasible. The CCSD(T) method for the same spin state and using the same basis set as in CI provides an approximation to the lowest eigenvalue of the CI matrix. Thus for a given basis set, absolute accuracy of CCSD(T) method for each spin state can be determined by comparing CCSD(T) energy against the lowest eigenvalue of the CI matrix.

Table S1 lists the absolute energies of the three terms obtained by full-valence (the core 1s electrons are not correlated) CI calculations with three different basis sets. Table S2 shows the absolute energies of the ^{3}P and ^{1}D states calculated with CCSD(T) method using three different basis sets.

Table S1. Full-valence CI absolute energies (hartrees) of the lowest three terms of carbon atom using three basis sets of increasing size

Basis set	$E_{electronic}$(AU)		
	^{3}P	^{1}D	^{1}S
6-311G(d,p)	-37.767049	-37.712809	-37.661885
cc-pVTZ	-37.781280	-37.732046	-37.679057
cc-pVQZ	-37.786813	-37.739354	-37.686958

Table S2. CCSD(T)-FC absolute energies (hartrees) for the lowest triplet and singlet terms of carbon atom versus basis set

Basis set	$E_{electronic}$(AU)	
	^{3}P	^{1}D
6-311G(d,p)	-37.766669	-37.708155
cc-pVTZ	-37.780762	-37.727207
cc-pVQZ	-37.786540	-37.734696

Full-CI and CCSD(T) energy differences being minor, in an absolute fashion is noteworthy and suggests a better performance of CCSD(T) on energy differences. Table S3 compares relative energies of the two singlets against the experimentally known values.

Table S3. Full-valence CI energies (kcal/mol) of the two lowest singlet terms relative to the ground term 3P of carbon atom versus basis set

Basis set	E_{rel} (kcal/mol)	
	^{1}D	^{1}S
6-311G(d,p)	34.0	66.0
cc-pVTZ	30.9	64.1
cc-pVQZ	29.8	62.7
Exp.	29.1	61.9

Use of cc-pVTZ basis set appears to produce sufficiently high quality results and the costly improvement achieved by employing cc-pVQZ may not be of interest depending on the system under study. Table S4 shows the absolute errors in the CCSD(T) energies as a function of basis set size.

Table S4. Difference (kcal/mol) between CCSD(T)-FC and CI-FC absolute energies for the lowest triplet and singlet terms of carbon atom versus basis set

Basis set	E_{rel} (kcal/mol)	
	^{3}P	^{1}D
6-311G(d,p)	0.24	2.92
cc-pVTZ	0.32	3.04
cc-pVQZ	0.17	2.92

It is seen that errors in both the singlet and triplet CCSD(T) values are nearly independent of basis set size. For the triplet, the CCSD(T) method almost exactly reproduces the computationally much more expensive CI results. Apparently the contribution of connected quadruple excitations (omitted in CCSD(T) formalism) to the energy of the triplet is not significant. On the other hand, the error of about 3 kcal/mol in the CCSD(T) values for the singlet state is attributable to these missing quadruple excitations. The improvement by using iterative instead of perturbative triple excitations and adding the connected quadruple excitations are given in Table S5.

Table S5. CCSD(T)-FC, CCSDT-FC, CCSDTQ-FC, and full-CI-FC energy comparison for C(^{1}D)

Method	^{1}D - $E_{electronic}$	Δ E_{rel} CCSD(T)	Δ E_{rel} full-CI
	(AU)	kcal/mol	
CCSD(T) /6-311G(d,p)	-37.708155	0.00	2.92
CCSDT/6-311G(d,p)	-37.708838	-0.43	2.49
CCSDTQ/6-311G(d,p)	-37.712809	-2.92	0.00

Assuming the carbon atom as a 4-electron system, the CCSD(T,FC) calculation on C(1D) is lacking only the contribution from the linked quadruple excitations. When the latter are included, i.e. CCSDTQ-FC,[a] the results of the CC method based on the (single-reference) RHF determinant is identical to those from a full-CI calculation, excluding the core electrons, full-CI-FC. The very minor difference of CCSD(T) and CCSDT energies are also noteworthy. Thus, the "best" result on absolute energies of carbon with the quality of full-CI will be via a CCSDTQ calculation and preferentially by employing a cc-pVQZ basis or higher. Given the unaffordable cost of such calculations for the C_2H_4O PES, one can either carry multi-configurational calculations where necessary (the initial phase on the singlet PES in this case) or verify the quality of the computed relative energies by referencing to experimental measurements as a result of successful systematic error cancellation in the CCSD(T) methodology. Note that the above errors are in absolute energies and a system dependent error cancellation can safely render CCSD(T) energies trustworthy.

II. Multi-reference Treatment of the Initial Species on the Singlet PES

Having studied the carbon atom electronic states, the question is whether or not an error cancellation of that sort is applicable to our system. To answer this we first point out that as long as a single

[a] CFOUR, a quantum chemical program package written by J.F. Stanton, J. Gauss, M.E. Harding, P.G. Szalay with contributions from A.A. Auer, R.J. Bartlett, U. Benedikt, C. Berger, D.E. Bernholdt, Y.J. Bomble, L. Cheng, O. Christiansen, M. Heckert, O. Heun, C. Huber, T.-C. Jagau, D. Jonsson, J. Jusélius, K. Klein, W.J. Lauderdale, D.A. Matthews, T. Metzroth, L.A. Mück, D.P. O'Neill, D.R. Price, E. Prochnow, C. Puzzarini, K. Ruud, F. Schiffmann, W. Schwalbach, S. Stopkowicz, A. Tajti, J. Vázquez, F. Wang, J.D. Watts and the integral packages *MOLECULE* (J. Almlöf and P.R. Taylor), *PROPS* (P.R. Taylor), *ABACUS* (T. Helgaker, H.J. Aa. Jensen, P. Jørgensen, and J. Olsen), and ECP routines by A. V. Mitin and C. van Wüllen.

reference description is suitable for a species, the question is obsolete. Secondly if two species on the PES incorporate a carbon atom that very much retains its ^{1}D character as an open shell singlet, the errors would be similar and the CCSD(T) performance on relative energies will be far better than that shown for absolute errors. Below we show that:

(i) Except for the CH insertion complex (**15**) and the subsequent TS (**15/16a**) none of the species on the initial entrance channel have any important multi-reference character.

(ii) **15** and **15/16a** posses a carbon atom that almost remains atomic in nature and the multi-reference electronic structure of these two species are originating from the carbon atom being very loosely bound to the system.

(iii) Relative energies of reactants ($C(^1D) + CH_3OH$) are much better computed by CCSD(T)/cc-pVTZ methodology than by different QDPT levels tested. This was indeed the case for $C(^1D) + H_2O$ system.

We carried various CASSCF and CAS-MP2 calculations on species **1**, **15**, **1/2**, **1/3**, **1/4**, and **15/16a**. We here report the more balanced CAS(8,8)-MP2 results for all six species (Table S6) and CAS(12,11)-MP2 results for the OH insertion channel (Table S7). Due to the more number of active orbitals and electrons required to describe the methyl fragment (all C–H bonds had to be considered) we could not fit the chemistry of interest for all the six species to a single active space larger than 8,8. When compared to experimental data, CCSD(T) relative energies were much better (~1 kcal/mol error) than QDPT energies.

Table S6. Energies, Leading CI coefficients and Natural Orbital Occupation Numbers (NOON) of Critical Orbitals for the Initial Species on the Singlet PES

	QDPT-i[a]	CCSD(T)[b]		Exp.				
Species	$E_{electronic}$(AU)	ΔH_{rel} (kcal(mol)			c_{CI}		NOON[d]	
C(^{1}D) + MeOH	-153.043349	183.6	191.0	192.0	0.68	-0.68	1.00	1.00
1	-153.064490	171.3	171.3	n/a	0.98	[c]	[e]	[f]
15	-153.057193	175.7	186.3	n/a	0.79	-0.58	1.30	0.70
1/2	-153.059031	173.3	169.8	n/a	0.98	[c]	[e]	[f]
1/3	-153.054680	173.9	169.2	n/a	0.98	[c]	[e]	[f]
1/4	-153.050640	177.8	177.0	n/a	0.98	[c]	[e]	[f]
15/16a	-153.055205	175.9	189.3	n/a	0.73	-0.66	1.09	0.91

[a]MCQDPT2/6-31G(d,p)//CAS(8,8)/6-31G(d,p), [b]cc-pVTZ/cc-pVTZ as reported in the discussion, [c]smaller than 0.1, [d]only the two MOs reported here are noteworthy as rest are all either doubly occupied (> 1.9) or unoccupied (< 0.1), [e] >1.9 [f] < 0.1.

Table S7. Comparison of Relative CCSD(T) Energies with QDPT Method Employing 8,8 and 12,11 Active Spaces in the CASSCF Reference

Species	QDPT-i[a]	QDPT-j[b]	CCSD(T)[c]	Exp.
	ΔH_{rel} (kcal(mol)			
C(1D) + MeOH	183.6	199.7	191.0	192.0
1	171.3	171.3	171.3	
15	175.7	n/a	186.3	
1/2	173.3	176.0	169.8	
1/3	173.9	172.1	169.2	
1/4	177.8	175.4	177.0	
15/16a	175.9	n/a	189.3	

[a]MCQDPT2/6-31G(d,p)//CAS(8,8)/6-31G(d,p), [b]MCQDPT2/6-31G(d,p)//CAS(12,11)/6-31G(d,p), [c]cc-pVTZ/cc-pVTZ as reported in the discussion.

All multi-reference calculations describe the early species on the OH-insertion channel with closed shell electronic structures. Particularly for complex **1** this result could be predicted by its tightly bound (C-O bond is1.453 Å) structure. Consequently CCSD(T)/cc-pVTZ relative energies are reliable for the closed shell species **1**, **1/2**, **1/3**, and **1/4**.

For **15** and **15/16a** the MCSCF expansion is dominated by two large configurations which are originating from the two singly occupied carbon atom *p* orbitals at infinite distance. (Almost) Singly occupied Natural Orbitals of **15** and **15/16a** are graphically visible as carbon *p* atomic orbitals. Taking into account the structurally loose natures of **15** and **15/16a** two results are clear:

(i) **15** and **15/16a** possess a loosely bound carbon atom that retains its atomic character (with two singly occupied *p* orbitals) which is the cause of the two large CI coefficients.

(ii) CCSD(T)/cc-pVTZ energies will still be reliable because of fortuitous error cancellation due to the very similar electronic structure of the two species.

Thus we can safely believe that the errors in the CCSD(T) energies of **15** and **15/16a** should be nearly the same (and in the same direction) as that in an isolated C(^{1}D) atom.

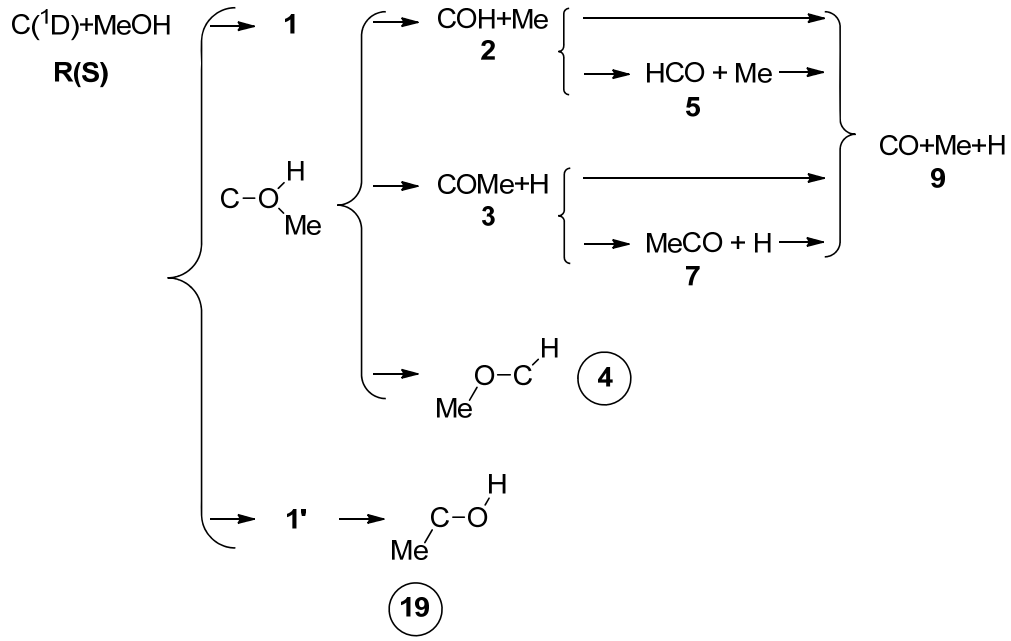
In addition, the reactivity scheme predicted by QDPT energies are qualitatively similar to those of CCSD(T), i.e. both CCSD(T) and QDPT computations predict that **1** and **15** can traverse their respective barriers to yield, **2**, **3**, **4**, and **16a** with low barriers. All these barriers are significantly lower than energy of the reactants. The only difference is in the prediction of existence of TSs **1/2** and **1/3** by QDPT, however this does not change the predictions on reaction products as QDPT barriers are very small. Moreover **1/2** and **1/3** do not need a multi-reference description as both are dominated by a single Slater determinant. Thus, based on CCSD(T) results these dissociation reactions are extremely facile. To better compute the barriers related with these two TSs we also performed CCSD(T)/6-311G(d,p) optimizations on **1**, **1/2**, and **1/3** and obtained essentially the same

result with CCSD optimizations. Both **1/2** and **1/3** are slightly (within a kcal/mol) over **1** on the electronic energy surface and lie below **1** after ZPVEs are added, hence dissociation products **2** and **3** are instantaneously generated on the attack of carbon to methanol.

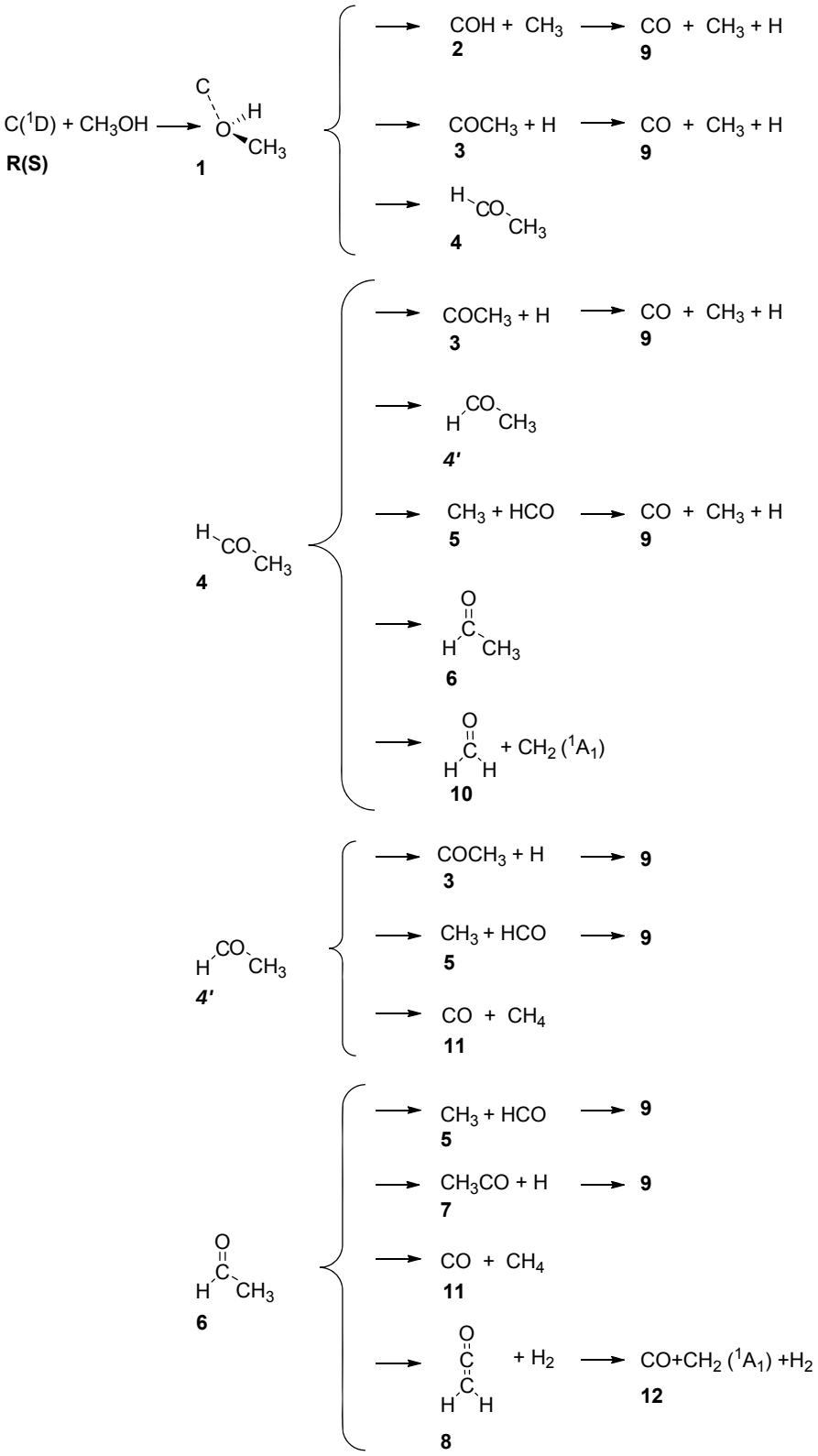
Table S8. Representation of the Singlet and Triplet Species Investigated

Label	Species
R(S)	$C(^1D)$+MeOH
R(T)	$C(^3P)$+MeOH
1	C--OHMe
1'	C--OHMe
2	COH+Me
3	COMe+H
4	Me-O-C-H
4'	cis-4
5	HCO+Me
6	MeCHO
7	MeCO+H
8	$H_2C=C=O+H_2$
9	CO+Me+H
10	$H_2C=O+CH_2$
11	$CO+CH_4$
12	$CO+H_2+CH_2$
13	$H_2C=CHOH$
14	$H_2O+C_2H_2$
15	$HO-CH_2$--H--C
16	$HO-CH_2$-C-H
17	H_2C-CH_2-O
18	$H_2C-O-CH_2$
19	Me-C-OH
20	H_2C-CHO+H
21	H_2C-C-OH+H
22	HC-CHOH+H
23	H_2C-OH+CH
24	H_2C-CH+OH
25	MeO+CH
26	$HC-O-CH_2+H$
27	H_2+HO-C=CH
28	Me-C+OH
29	$c-CH_2CO+H_2$
30	$CHCHO+H_2$
31T	$O(^3P)+C_2H_4$

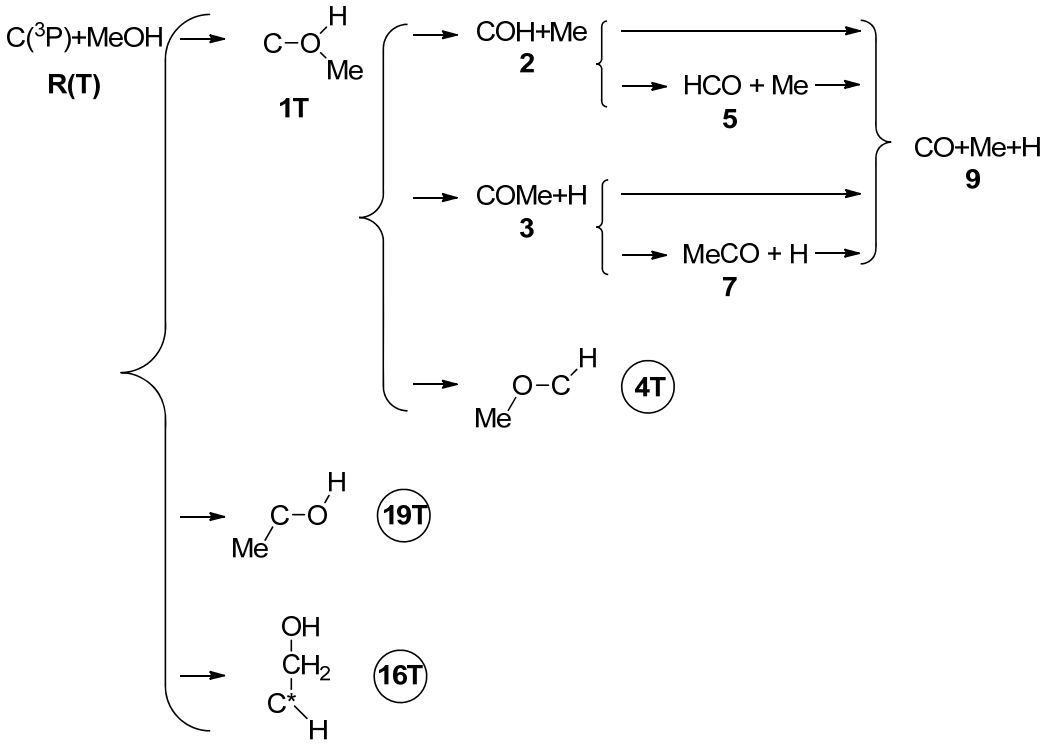
Scheme S1. Initial Exit Channels from **1** and **1'**



Scheme S2. Reaction Paths and Species on the Singlet PES



Scheme S3. Initial Exit Channels from **1T**



Scheme S4. Reaction Paths and Species on the Triplet PES

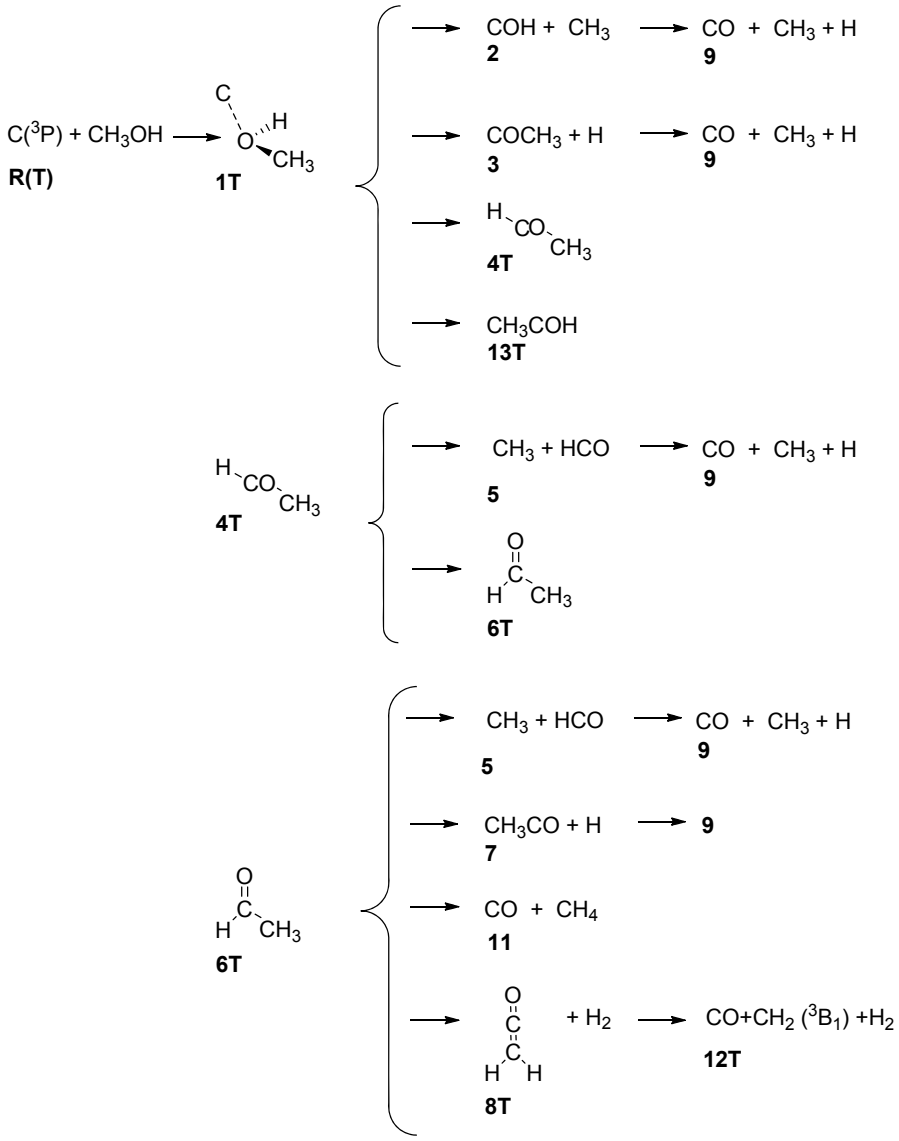


Table S9. Relative Enthalpies (kcal/mol) of C_2H_4O Isomers at 0K[a]

	CCSD(T)/ 6-311G(d,p)	CCSD(T)/ cc-pVTZ	EXP[b]
R(S)	191.1	191.0	192.0
1	177.9	176.4	
2	119.6	121.6	
3	139.4	141.9	
4	67.4	67.1	
4'	71.5	70.6	
5	78.0	80.3	84.0
6	0.0	0.0	0.0
7	83.7	86.6	
8	25.2	26.0	27.6
9	87.2	93.3	98.5
10	111.5	112.1	115.5
11	-12.2	-8.3	-4.8
12	103.6	108.4	104.3
13	12.8	10.5	10.2[c] (298K)
14	39.1	36.9	35.7
1/2	171.4	169.8	
2/9	124.6	127.6	
1/3	170.2	169.2	
3/9	139.2	142.2	
1/4	179.2	177.0	
4/5	85.8	88.7	
4/6	115.9	114.0	
4/4'	97.9	96.6	
4'/5	83.3[d]		
4'/11	85.6	87.6	
6/11	82.8	82.8	
6/8	83.2	81.2	
5/9	93.0	97.6	
7/9	97.1	101.6	
13/6	69.3	67.1	
13/14	92.2	89.6	
R(T)	154.4	157.4	162.8
1T	144.2	146.1	
4T	93.8	94.1	
6T	75.8	76.9	
1T/2	162.2	162.6	
1T/3	170.9	171.4	
1T/4T	158.7	158.5	
1T/13T	179.1	177.6	
4T/5	107.3	108.1	
4T/6T	136.8	135.6	
6T/5	89.9	90.6	
6T/7	95.0	96.3	

[a] All values are relative to CH_3CHO ($^1A'$)
[b] Data taken from Computational Chemistry Comparison and Benchmark Database (CCCBDB) at http://srdata.nist.gov/cccbdb/default.htm.
[c] ΔH_{298}
[d] Rel. to 4' at MCQDPT(2,2)/6-31G(d,p) level (optimization and frequency calculations) with active orbital (may be called HOMO & LUMO) occupancies of η_{12} =1.699 and η_{13}=0.301 respectively. RCCSD can not locate a TS, and departs the fragments as neutral methyl and formyl radicals.

Table S10. Relative 0K Enthalpies of the Singlet Minima at Various Theoretical Levels as Specified

Label	Species	Point group	CCSD 6-311G (d,p)	CCSD(T) 6-311G (d,p)	CCSD cc-pVTZ	CCSD(T) cc-pVTZ
R(S)	$C(^1D)$+MeOH	C_s	188.4	191.1	188.3	191.0
1	C--OHMe	C_s	172.7	173.5	170.7	171.3
1'	C--OHMe	C_1	177.3	177.9	175.8	176.4
2	COH+Me	C_s+D_{3h}	116.8	119.6	118.5	121.6
3	COMe+H	C_s, $^2A'$	138.5	139.3	140.8	141.8
4	Me-O-C-H	C_s	67.0	67.4	66.8	67.1
4'	cis-4	C_s	71.4	71.5	70.5	70.6
5	HCO+Me	C_s+D_{3h}	76.8	78.0	78.8	80.3
6 (Ref)	MeCHO	C_s	0.0	0.0	0.0	0.0
7	MeCO+H	C_s, 2A'	83.8	83.5	86.6	86.5
8	H_2C=C=O+H_2	C_{2v}	26.7	25.2	27.4	26.0
9	CO+Me+H		86.1	87.1	91.7	93.2
10	H_2C=O+CH2($^1A_1$)	C_{2v}	110.0	111.5	110.4	112.1
11	CO+CH_4		-12.4	-12.2	-8.9	-8.3
12	CO+H_2+CH_2	$CH_2(^1A_1)$	102.7	103.6	106.9	108.4
13	H_2C=CHOH	C_s	12.8	12.9	10.7	10.5
14	H2O+C_2H_2		38.9	39.1	37.0	36.9
15	HO-CH_2--H--C	C_1	187.9	187.5	186.6	186.3
16a	HO-CH_2-C-H	C_s	91.2	92.7	88.8	90.2
16b	HO-CH_2-C-H	C_1	95.5	95.5	93.7	93.3
17	H_2C-CH_2-O	C_{2v}	30.1	30.2	28.1	28.1
19	Me-C-OH	C_s	50.3	50.8	50.2	50.7
20	H_2C-CHO+H	C_s, $^2A''$	90.3	91.3	91.9	93.1
21	H_2C-C-OH+H	C_1, ^2A	116.3	116.7	117.1	117.5
22	HC-CHOH+H	C_s, $^2A'$	120.2	120.9	120.7	121.4
23	H_2C-OH+CH	C_1, ^2A	168.3	172.2	169.2	173.4
24	H_2C-CH+OH	C_s, $^2A'$	112.3	115.4	113.2	116.5
25	MeO+CH	C_s, $^2A'$	174.1	178.8	176.2	181.2
26	HC-O-CH_2+H	C_s, $^2A''$	162.2	163.1	163.8	164.8
27	H_2+HO-C=CH	C_s, $^1A'$	61.4	60.6	61.2	60.3

All the values are relative to singlet formaldehyde and in kcal/mol.

Table S11. Relative 0K Enthalpies of the Singlet TSs at Various Theoretical Levels as Specified

Label	Point group	CCSD 6-311G (d,p)	CCSD(T) 6-311G (d,p)	CCSD cc-pVTZ	CCSD(T) cc-pVTZ
1/19		196.0	193.6	193.4	190.7
1/2		172.7	171.4	171.2	169.8
1/3		172.4	170.2	171.4	169.2
1/4		179.9	179.2	178.0	177.0
2/9		123.4	124.6	126.2	127.6
3/9	C_s	139.4	139.1	142.4	142.1
4/5	C_s	107.0	85.8	109.6	88.7
4/4'	C_1	96.8	97.9	95.6	96.6
4/6	C_1	117.7	115.9	116.1	114.0
4/10	C_s	116.6	114.3	116.3	113.7
4'/11	C_s	102.4	85.6	104.4	87.6
5/9		92.4	93.0	96.5	97.5
6/8	C_1	87.5	83.2	85.8	81.2
6/11	C_s	86.6	82.8	86.9	82.8
6/13	C_1	72.1	69.3	70.2	67.1
6/19	C_s	82.8	80.4	81.6	79.1
13/14		94.5	92.2	92.4	89.7
7/9		97.4	97.0	101.7	101.5
15/16a		188.9	190.0	188.4	189.3
16a/16b		97.9	99.3	96.4	97.7
16a/27		131.1	129.7	128.3	126.4
16b/17		100.5	98.1	98.9	96.1

All the values are relative to singlet formaldehyde and in kcal/mol.

Table S12. Relative 0K Enthalpies of the Triplet Minima[a]

Label	Species	CCSD(T) 6-311G (d,p)	CCSD(T) cc-pVTZ	EXP.[b]
R(T)	$C(^3P)$+MeOH	154.4	157.4	162.8
1T	C--OHMe	144.2	146.1	
4T	Me-O-C-H	93.8	94.1	
6T	MeCHO	75.8	76.9	
10T	H_2C=O+$CH_2(^3B_1)$	99.4	102.2	
13T	H_2C=CHOH	77.3	76.6	
15T	HO-CH_2--H--C	154.8	158.9	
16T	HO-CH_2-C-H	88.7	89.0	
17T	H_2C-CH_2-O	84.6	85.2	
18T	H_2C-O-CH_2	88.0	87.1	
19T	Me-C-OH	79.8	80.4	

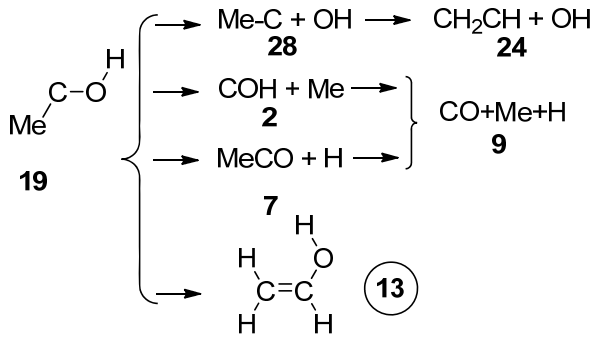
[a] All the values are relative to singlet acetaldehyde and in kcal/mol.
[b] Data taken from Computational Chemistry Comparison and Benchmark Database (CCCBDB) at http://srdata.nist.gov/cccbdb/default.htm.

Table S13. Relative 0K Enthalpies of the Triplet TSs[a]

Label	CCSD(T) 6-311G (d,p)	CCSD(T) cc-pVTZ
15T/16T	159.7	159.2
1T/19T	179.1	177.7
1T/2	162.2	162.6
1T/3	171.1	171.5
1T/4T	158.7	158.5
4T/5	107.3	108.1
4T/6T	136.8	135.6
4T/18T	129.6	128.9
6T/5	89.9	90.6
6T/7	95.0	96.3
6T/13T	110.5	109.6
6T/17T	118.5	117.7
13T/19T	128.5	127.2
13T/16T	132.1	130.7
18T/10T	119.1	120.0
17T/10T	107.9	108.8

[a] All the values are relative to singlet acetaldehyde and in kcal/mol.

Scheme S5. Reactions of **19**



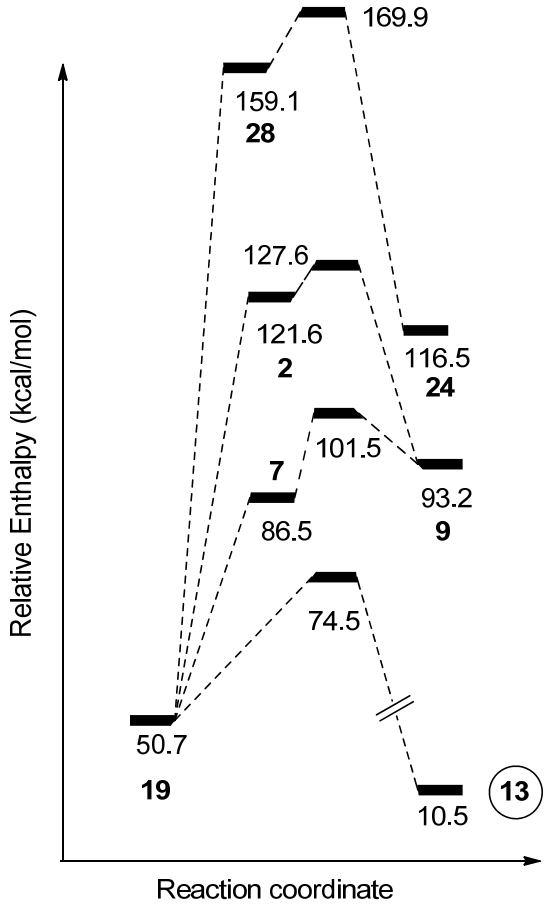
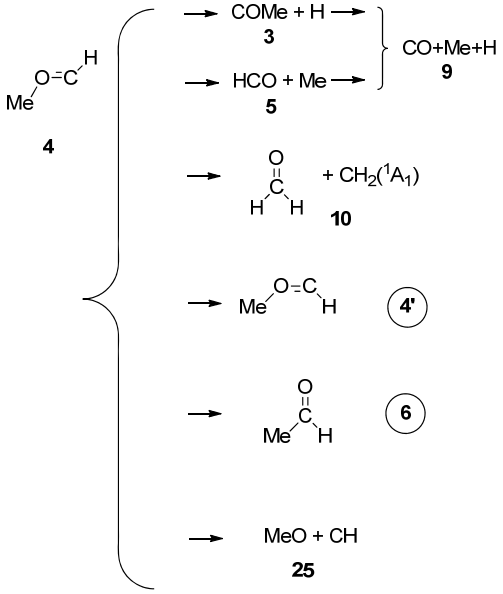


Figure S1. Relative 0K enthalpy (ΔH_0) profile for reactions of singlet carbene **19**.
Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S6. Reactions of **4**



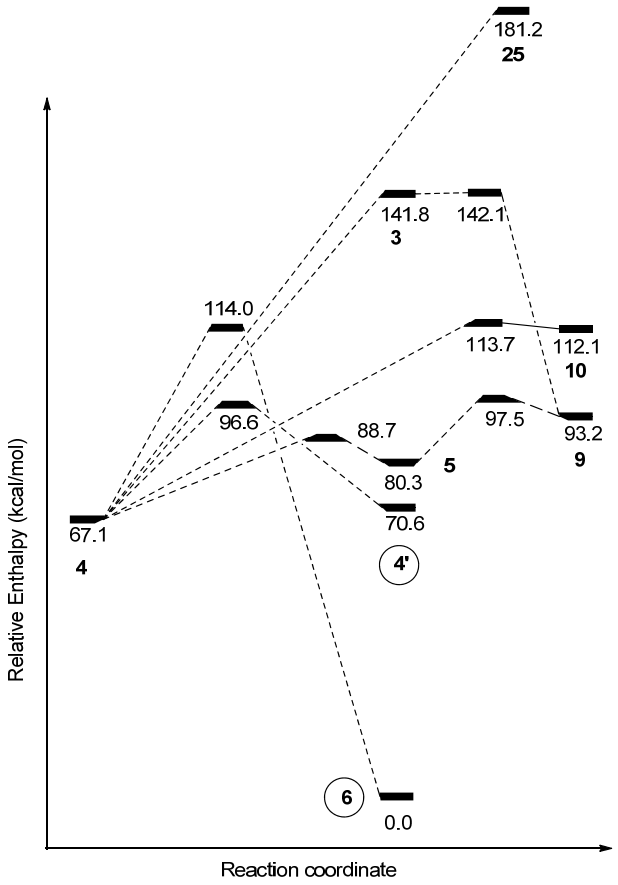
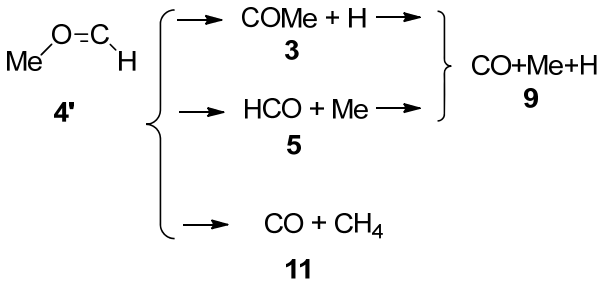


Figure S2. Relative 0K enthalpy (ΔH_0) profile for reactions of singlet trans-methoxycarbene **4**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S7. Reactions of **4'**



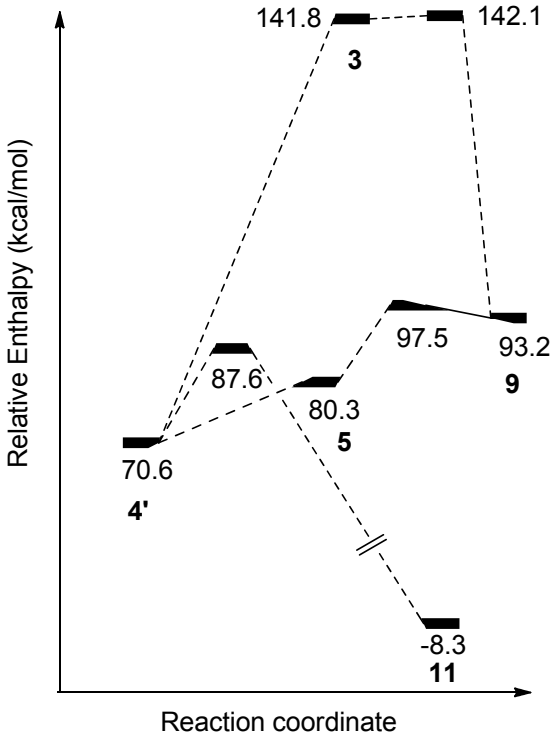
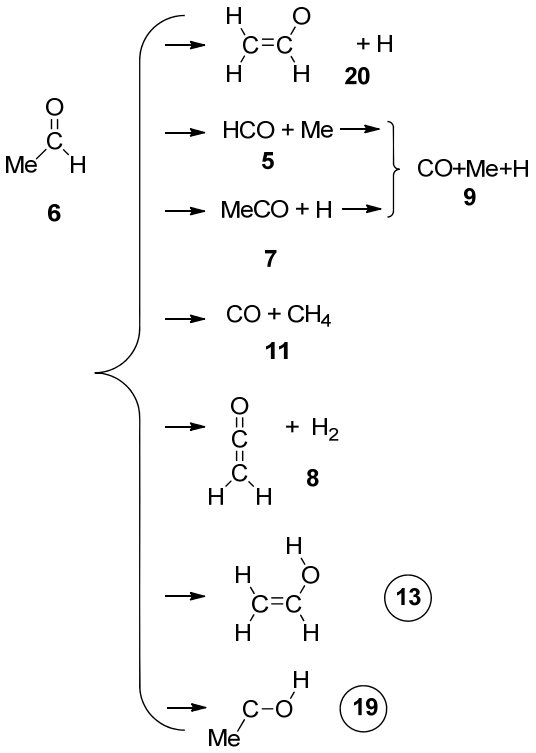


Figure S3. Relative 0K enthalpy (ΔH_0) profile for reactions of singlet carbene cis-methoxymethylene **4'**.
Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S8. Reactions of **6**



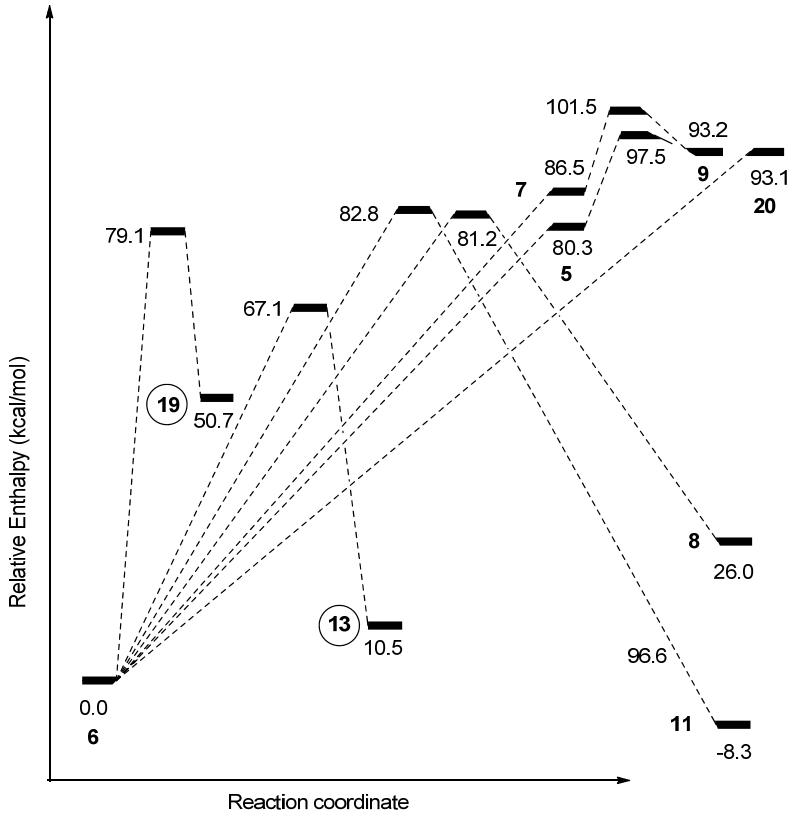
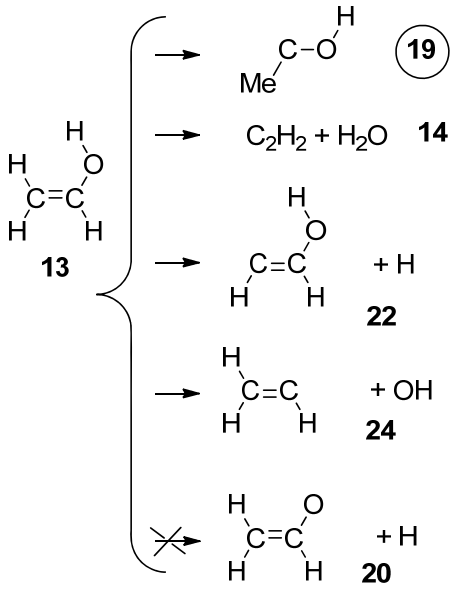


Figure S4. Relative 0K enthalpy (ΔH_0) profile for reactions of singlet acetaldehyde **6**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S9. Reactions of **13**



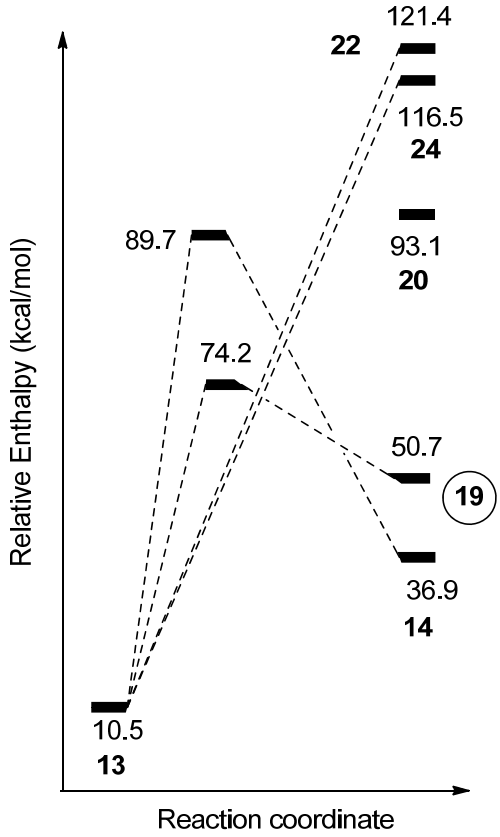
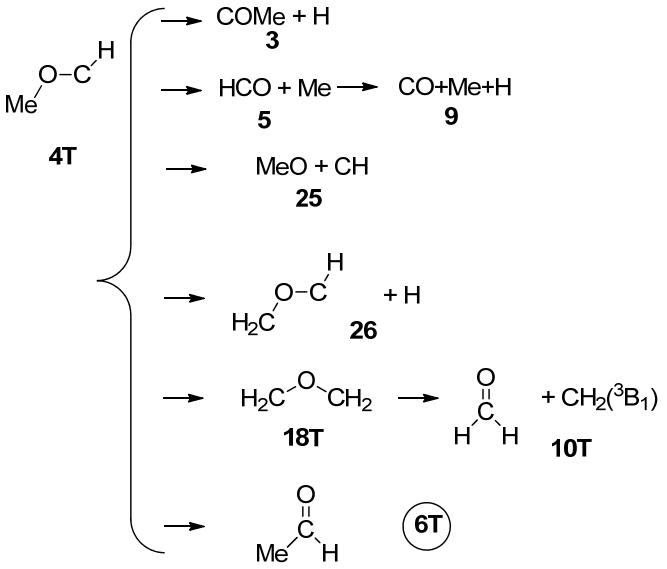


Figure S5. Relative 0K enthalpy (ΔH_0) profile for reactions of singlet vinyl alcohol (ethanol) **13**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S10. Reactions of **4T**



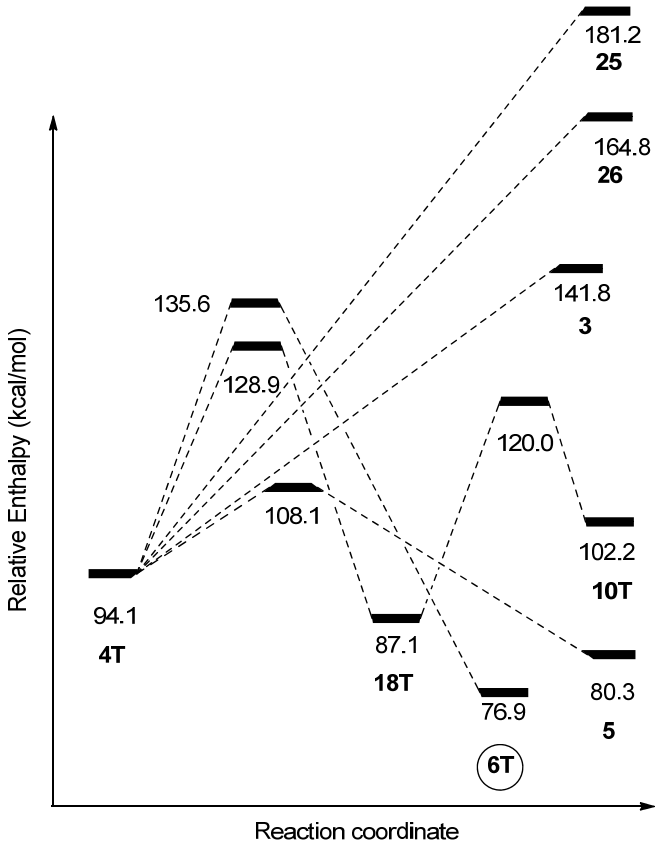
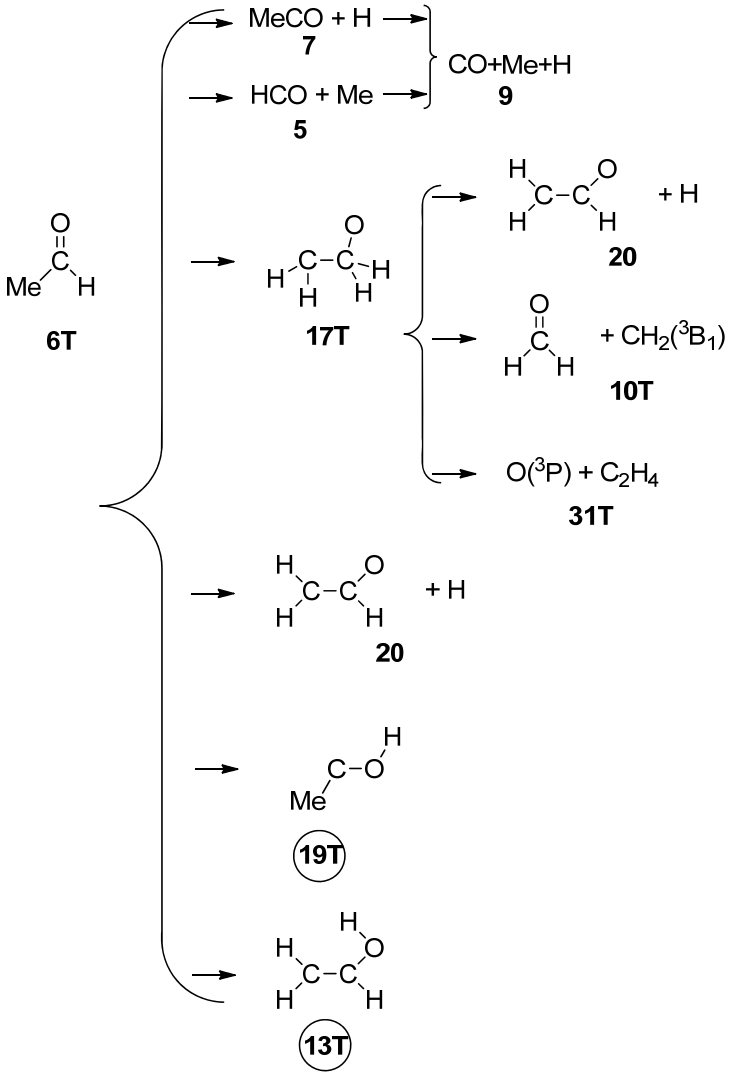


Figure S6. Relative 0K enthalpy (ΔH_0) profile for reactions of triplet methoxymethylene **4T**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S11. Reactions of **6T**



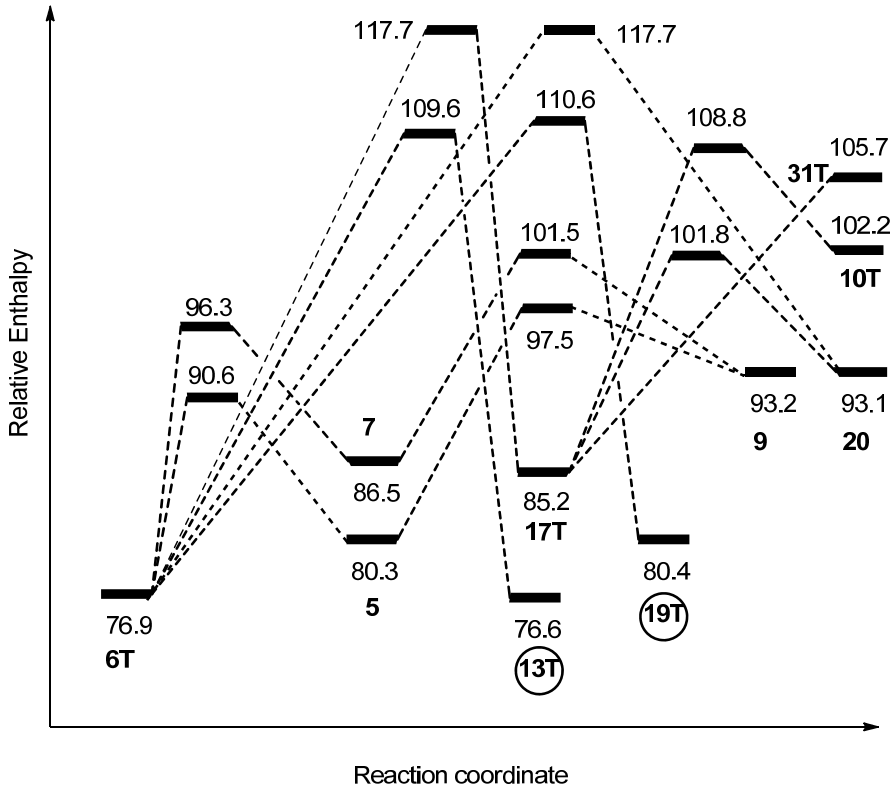
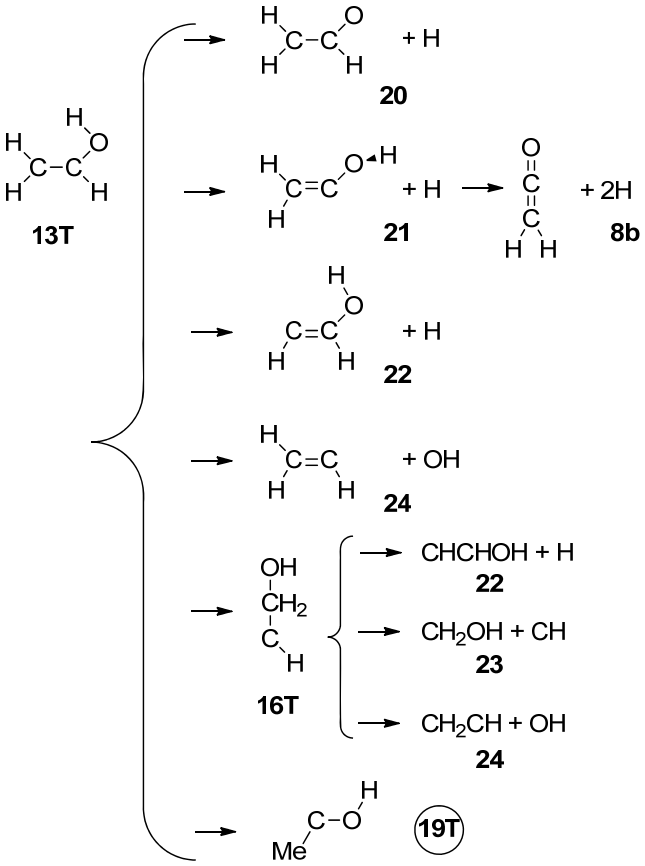


Figure S7. Relative 0K enthalpy (ΔH_0) profile for reactions of triplet acetaldehyde **6T**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S12. Reactions of **13T**



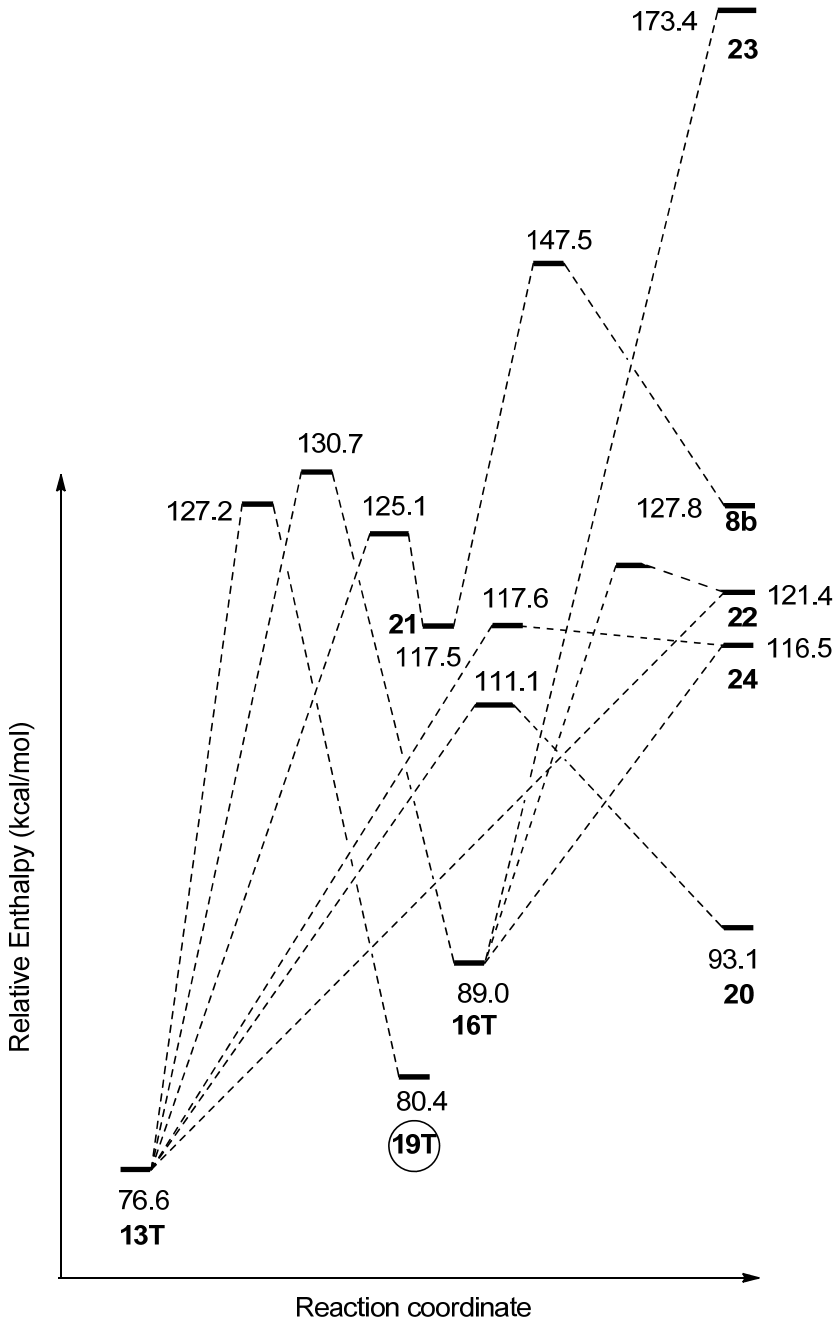
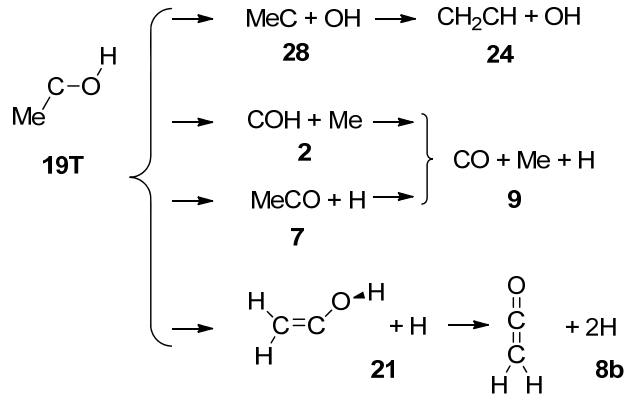


Figure S8. Relative 0K enthalpy (ΔH_0) profile for reactions of triplet CH_2CHOH **13T**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S13. Reactions of **19T**



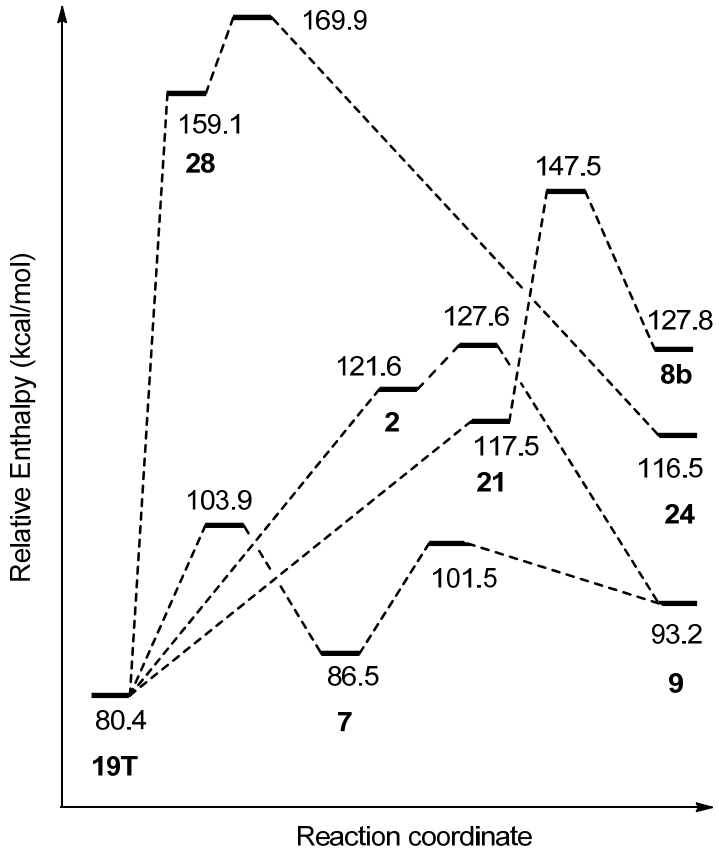
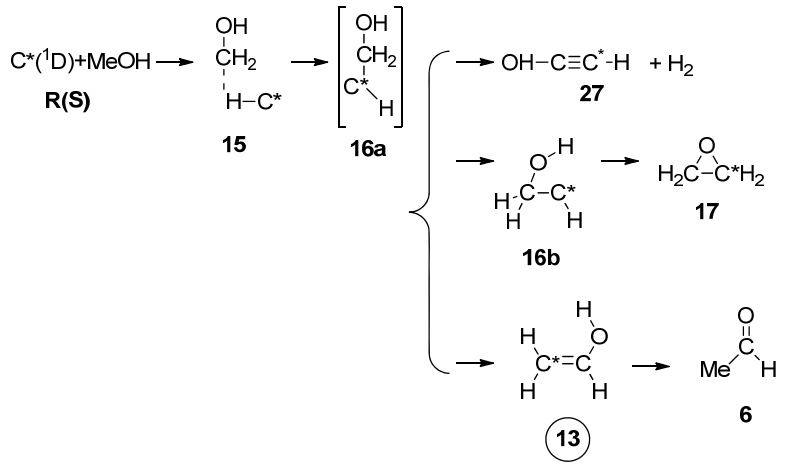


Figure S9. Relative 0K enthalpy (ΔH_0) profile for reactions of triplet O–C insertion carbene **19T**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S14. Formation of **13** on the Singlet C–H Insertion Path



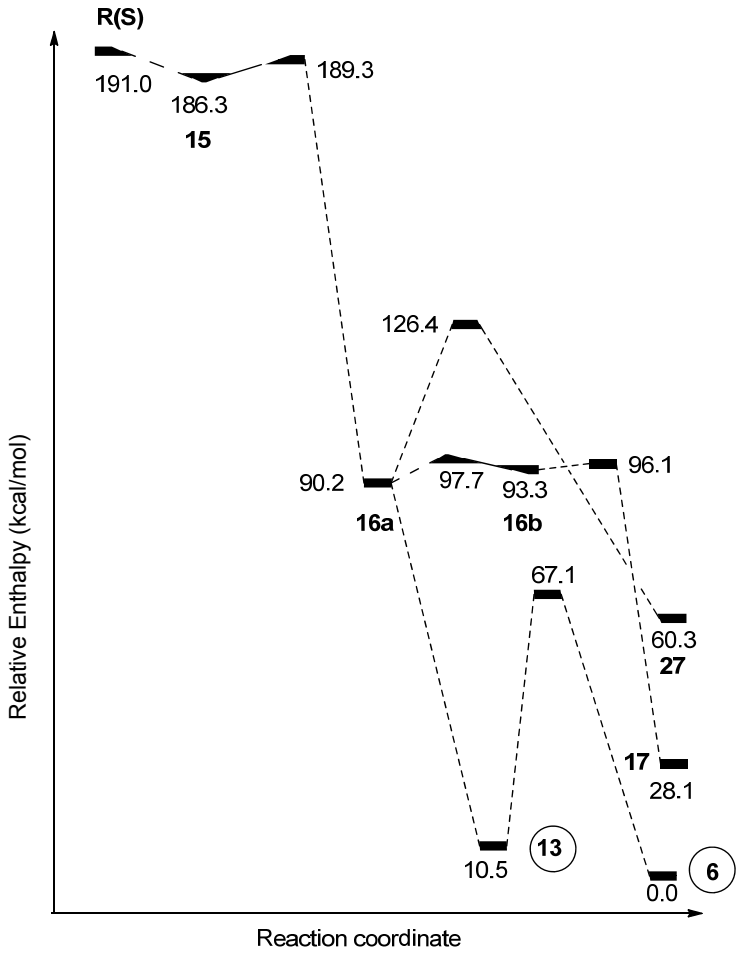
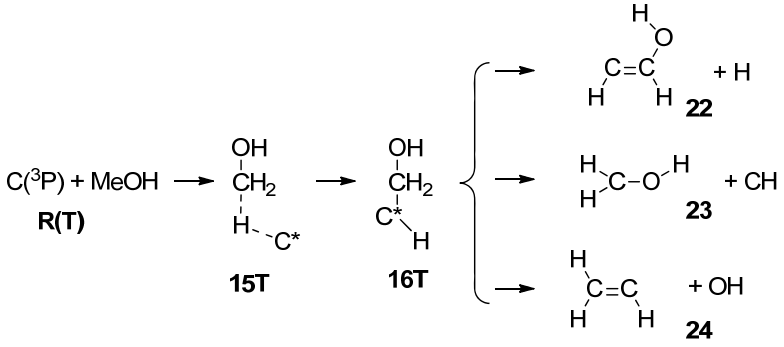


Figure S10. Relative 0K enthalpy (ΔH_0) profile for reactions of singlet C–H insertion complex **15**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Scheme S15. Exit Channels from Triplet C–H Insertion Product **15T**



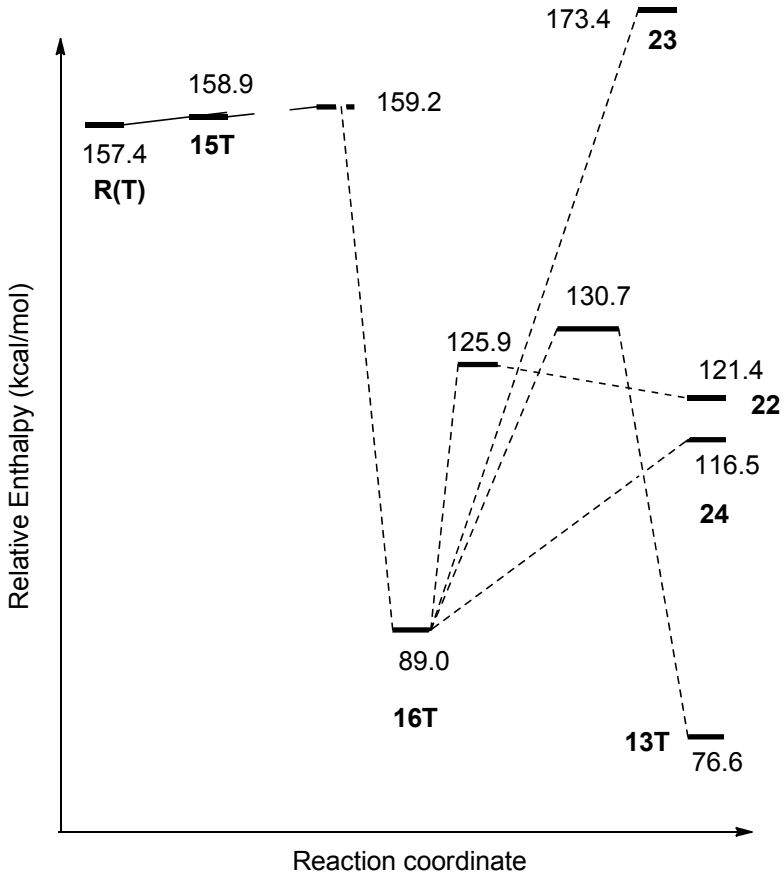


Figure S11. Relative 0K enthalpy (ΔH_0) profile for reactions of triplet C–H insertion complex **15T**. Energies are relative to acetaldehyde (species **6**) calculated at CCSD(T)/cc-pVTZ//CCSD/6-311g(d,p) level.

Table S14. Coupled Cluster Total Electronic Energies (Hartree) of Singlet Minima

Label	Species	E (AU) CCSD/ 6-311G(d,p)	E (AU) CCSD(T)/ 6-311G(d,p)	E (AU) CCSD/ cc-pVTZ	E (AU) CCSD(T)/ cc-pVTZ
R(S)	$C(^1D)$+MeOH	-153.162928	-153.176785	-153.258141	-153.277931
1	C--OHMe	-153.189471	-153.206336	-153.287649	-153.310801
1'	C--OHMe	-153.184040	-153.201213	-153.281350	-153.304596
2	COH+Me	-153.268597	-153.282366	-153.360853	-153.380105
3	COMe+H	-153.234004	-153.250843	-153.325227	-153.347814
4	Me-O-C-H	-153.359950	-153.377530	-153.455299	-153.478869
4'	cis-4	-153.352421	-153.370355	-153.448732	-153.472724
5	HCO+Me	-153.331586	-153.347813	-153.423268	-153.445003
6	MeCHO	-153.467139	-153.485322	-153.562130	-153.586240
7	MeCO+H	-153.321090	-153.339645	-153.411554	-153.435863
8	$H_2C=C=O+H_2$	-153.410368	-153.431040	-153.504262	-153.530642
8b	$H_2C=C=O$+2H	-153.242027	-153.262699	-153.331926	-153.358305
9	CO+Me+H	-153.308630	-153.325155	-153.394748	-153.416449
10	$H_2C=O+CH_2(^1A_1)$	-153.279330	-153.295212	-153.373754	-153.395169
11	$CO+CH_4$	-153.481011	-153.498766	-153.570296	-153.593565
12	$CO+H_2+CH_2$	-153.279214	-153.295969	-153.367390	-153.389190
13	$H_2C=CHOH$	-153.447671	-153.465611	-153.545924	-153.570393
14	$H_2O+C_2H_2$	-153.397495	-153.415438	-153.495632	-153.519822
15	$HO-CH_2$--H--C	-153.165107	-153.183815	-153.262046	-153.286603
16a	$HO-CH_2$-C-H	-153.317954	-153.333706	-153.416645	-153.438568
16b	$HO-CH_2$-C-H	-153.314440	-153.332671	-153.412354	-153.436965
17	H_2C-CH_2-O	-153.421373	-153.439349	-153.519415	-153.543605
19	Me-C-OH	-153.386869	-153.404156	-153.481973	-153.505277
20	H_2C-CHO+H	-153.309830	-153.326330	-153.402175	-153.424473
21	H_2C-C-OH+H	-153.269297	-153.286827	-153.362910	-153.386480
22	HC-CHOH+H	-153.263007	-153.280067	-153.357110	-153.380193
23	H_2C-OH+CH	-153.187433	-153.199371	-153.280958	-153.298381
24	H_2C-CH+OH	-153.277508	-153.290839	-153.371038	-153.389889
25	MeO+CH	-153.177362	-153.188134	-153.269156	-153.285154
26	HC-O-CH_2+H	-153.192970	-153.209769	-153.285348	-153.307935
27	H_2+HO-C=CH	-153.355284	-153.374845	-153.450670	-153.476263
28	Me-C+OH	-153.203568	-153.214862	-153.295880	-153.312547
29	c-CH_2CO+H_2	-153.315249	-153.335542	-153.408770	-153.434873
30	$CHCHO+H_2$	-153.280305	-153.303282	-153.375428	-153.404009

Table S15. B3LYP Total Electronic Energies (Hartree) of Singlet Minima

Label	Species	E (AU) B3LYP/6-311G(d,p)
2	COH+Me	-153.673366
3	COMe+H	-153.637311
4	Me-O-C-H	-153.767885
4'	cis-4	-153.761188
5	HCO+Me	-153.740352
6	MeCHO	-153.876861
7	MeCO+H	-153.726772
8	$H_2C=C=O+H_2$	-153.827324
9	CO+Me+H	-153.699993
10	$H_2C=O+CH_2(^1A_1)$	-153.680699
11	$CO+CH_4$	-153.879983
12	$CO+H_2+CH_2$	-153.670164
13	$H_2C=CHOH$	-153.856733
14	$H_2O+C_2H_2$	-153.802146
16a	$HO-CH_2-C-H$	-153.727844
16b	$HO-CH_2-C-H$	-153.722981
17	H_2C-CH_2-O	-153.830129
19	Me-C-OH	-153.794391
20	$H_2C-CHO+H$	-153.716865
21	$H_2C-C-OH+H$	-153.676990
22	HC-CHOH+H	-153.669026
23	$H_2C-OH+CH$	-153.587579
24	$H_2C-CH+OH$	-153.681560
25	MeO+CH	-153.578098
26	$HC-O-CH_2+H$	-153.598193
27	$H_2+HO-C=CH$	-153.767053
28	Me-C+OH	-153.604104
29	$c-CH_2CO+H_2$	-153.721261
30	$CHCHO+H_2$	-153.698791
8b	$H_2C=C=O+2H$	-153.647753

Table S16. Coupled Cluster Total Electronic Energies (Hartree) of Triplet Minima

Label	Species	E (AU) CCSD/ 6-311G(d,p)	E (AU) CCSD(T)/ 6-311G(d,p)	E (AU) CCSD/ cc-pVTZ	E (AU) CCSD(T)/ cc-pVTZ
R(T)	$C(^3P)$+MeOH	-153.224023	-153.235298	-153.314659	-153.331487
1T	C--OHMe	-153.239589	-153.253691	-153.331323	-153.351546
4T	Me-O-C-H	-153.318921	-153.333763	-153.413515	-153.434265
6T	MeCHO	-153.347683	-153.362150	-153.441096	-153.461314
10T	H_2C=O+$CH_2(^3B_1)$	-153.300575	-153.315189	-153.391669	-153.411648
13T	H_2C=CHOH	-153.344593	-153.359042	-153.440684	-153.461056
15T	HO-CH_2--H--C	-153.224825	-153.236280	-153.313601	-153.330679
16T	HO-CH_2-C-H	-153.328488	-153.342356	-153.422960	-153.442735
17T	H_2C-CH_2-O	-153.333025	-153.346180	-153.427335	-153.446158
18T	H_2C-O-CH_2	-153.326692	-153.341417	-153.423023	-153.443644
19T	Me-C-OH	-153.341992	-153.356547	-153.436018	-153.456492
31T	$O(^3P)$+C_2H_4	-153.305131	-153.318008	-153.394853	-153.412720

Table S17. B3LYP Total Electronic Energies (Hartree) of Triplet Minima

Label	Species	E (AU) B3LYP/6-311G(d,p)
R(T)	$C(^3P)$+MeOH	-153.613383
1T	C--OHMe	-153.640923
4T	Me-O-C-H	-153.727712
6T	MeCHO	-153.759860
10T	H_2C=O+$CH_2(^3B_1)$	-153.689827
13T	H_2C=CHOH	-153.755497
15T	HO-CH_2--H--C	-153.622721
16T	HO-CH_2-C-H	-153.727444
17T	H_2C-CH_2-O	-153.742958
18T	H_2C-O-CH_2	-153.738603
19T	Me-C-OH	-153.749467
31T	$O(^3P)$+C_2H_4	-153.699364

Table S18. Coupled Cluster Total Electronic Energies (Hartree) of Singlet TSs

Label	E (AU) CCSD/ 6-311G(d,p)	E (AU) CCSD(T)/ 6-311G(d,p)	E (AU) CCSD/ cc-pVTZ	E (AU) CCSD(T)/ cc-pVTZ
1/19	-153.149100	-153.171115	-153.248250	-153.276596
1/2	-153.187191	-153.207362	-153.284468	-153.310811
1/3	-153.184294	-153.205893	-153.280817	-153.308450
1/4	-153.174556	-153.193911	-153.272562	-153.298257
2/9	-153.250589	-153.266881	-153.341111	-153.363014
3/9	-153.229268	-153.247999	-153.319445	-153.344065
4/5	-153.288299	-153.340353	-153.379143	-153.436629
4/4'	-153.309348	-153.325844	-153.406340	-153.428888
4/6	-153.275720	-153.296762	-153.373122	-153.400628
4/10	-153.275156	-153.296989	-153.370624	-153.398764
4'/11	-153.296384	-153.341345	-153.388250	-153.438991
5/9	-153.299437	-153.316575	-153.387809	-153.410303
6/8	-153.318660	-153.343666	-153.416407	-153.447757
6/11	-153.322641	-153.346911	-153.417226	-153.447844
6/13	-153.347005	-153.369737	-153.445019	-153.474165
6/19	-153.329154	-153.351128	-153.425947	-153.454115
13/14	-153.310857	-153.332699	-153.409078	-153.437612
7/9	-153.294687	-153.313424	-153.382796	-153.407179
15/16a	-153.161801	-153.178227	-153.257541	-153.280175
16a/16b	-153.308648	-153.324589	-153.406067	-153.428159
16a/27	-153.249392	-153.269826	-153.348876	-153.375949
16b/17	-153.303203	-153.325188	-153.400847	-153.429315
28/24	-153.186468	-153.200640	-153.280205	-153.299948
21/8b	-153.208353	-153.229336	-153.301404	-153.328551

Table S19. B3LYP Total Electronic Energies (Hartree) of Singlet TSs

Label	E (AU) B3LYP/6-311G(d,p
1/3	-153.604981
2/9	-153.662728
3/9	-153.636823
4/5	-153.725230
4/4'	-153.718445
4/6	-153.689872
4/10	-153.690943
4'/11	-153.712126
4'/5	-153.733179
5/9	-153.701058
6/8	-153.743420
6/11	-153.743272
6/13	-153.765948
6/19	-153.743328
13/14	-153.727943
7/9	-153.696238
16a/16b	-153.713697
16a/27	-153.669980
16b/17	-153.714694
28/24	-153.591389
21/8b	-153.630064

Table S20. Coupled Cluster Total Electronic Energies (Hartree) of Triplet TSs

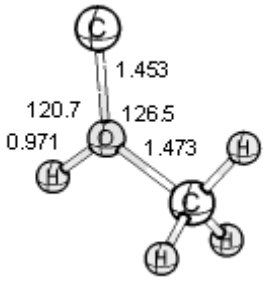
Label	E (AU) CCSD/ 6-311G(d,p)	E (AU) CCSD(T)/ 6-311G(d,p)	E (AU) CCSD/ cc-pVTZ	E (AU) CCSD(T)/ cc-pVTZ
15T/16T	-153.207121	-153.224372	-153.302428	-153.326036
1T/19T	-153.176344	-153.195441	-153.273000	-153.298649
1T/2	-153.203223	-153.221418	-153.297103	-153.321709
1T/3	-153.185039	-153.203851	-153.278935	-153.304046
1T/4T	-153.207163	-153.225628	-153.301974	-153.326828
4T/5	-153.289502	-153.307455	-153.382996	-153.407208
4T/6T	-153.243711	-153.262304	-153.340249	-153.365196
4T/18T	-153.253789	-153.271094	-153.349524	-153.373052
6T/5	-153.316959	-153.334962	-153.410691	-153.434765
6T/7	-153.305027	-153.323870	-153.397752	-153.422633
6T/13T	-153.283845	-153.301938	-153.379933	-153.404357
6T/17T	-153.270632	-153.288623	-153.366510	-153.390801
6T/19T	-153.284097	-153.301696	-153.379491	-153.403296
13T/19T	-153.256460	-153.273435	-153.353256	-153.376521
13T/16T	-153.250680	-153.267026	-153.347583	-153.370168
18T/10T	-153.269993	-153.286391	-153.363366	-153.385864
17T/10T	-153.289732	-153.305107	-153.383279	-153.404526
17T/20	-153.296631	-153.312434	-153.391151	-153.412885
13T/20	-153.277311	-153.295997	-153.372794	-153.397679
13T/21	-153.255719	-153.274165	-153.351110	-153.375636
13T/24	-153.272981	-153.289837	-153.368586	-153.391614
19T/7	-153.292933	-153.311208	-153.385964	-153.410428
16T/22	-153.256238	-153.273207	-153.351698	-153.374774

Table S21. B3LYP Total Electronic Energies (Hartree) of Triplet TSs

Label	E (AU) B3LYP/6-311G(d,p
15T/16T	-153.617471
1T/19T	-153.592482
1T/2	-153.621172
1T/3	-153.604213
1T/4T	-153.617975
4T/5	-153.709839
4T/6T	-153.660243
4T/18T	-153.667597
6T/5	-153.734674
6T/7	-153.720394
6T/13T	-153.701778
6T/17T	-153.692126
6T/20	-153.691058
6T/19T	-153.698396
13T/19T	-153.672513
13T/16T	-153.664698
18T/10T	-153.685823
17T/10T	-153.698519
17T/20	-153.711699
13T/20	-153.699055
13T/21	-153.671869
13T/24	-153.689901
19T/7	-153.712445
16T/22	-153.669376

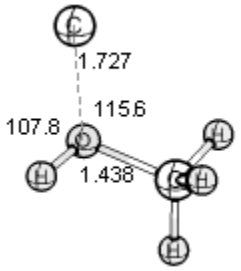
CCSD/6-311G(d,p) OPTIMIZED GEOMETRIES AND CARTESIAN COORDINATES

The structures below are given in the order:
1) Minima on the singlet PES
2) Transition structures on the singlet PES, magnitude of imaginary frequency included.
3) Minima on the triplet PES
4) Transition structures on the triplet PES, magnitude of imaginary frequency included.
5) Radicalic species located as minima



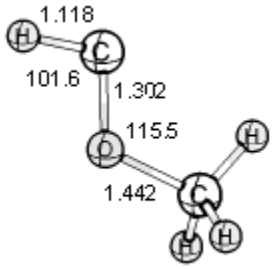
1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.452648000	0.466130000	0.000000000
8	0.000000000	0.441546000	0.000000000
6	-0.856651000	-0.756650000	0.000000000
1	-0.510004000	1.267348000	0.000000000
1	-0.129260000	-1.566016000	0.000000000
1	-1.468359000	-0.745291000	0.905384000
1	-1.468359000	-0.745291000	-0.905384000



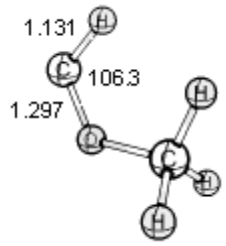
1′

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.00000000	0.00000000	0.00000000
8	0.00000000	0.00000000	1.72747400
6	1.29695100	0.00000000	2.34941700
1	1.18001200	0.00000000	3.43495200
1	1.84765700	0.89146400	2.04269700
1	1.88140000	-0.74402900	1.80453000
1	-0.56615100	0.64099500	2.16686700



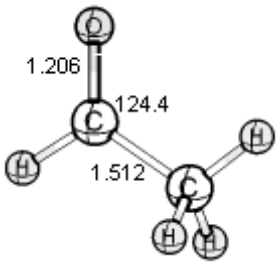
4

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.109984000	0.135101000	-0.000010000
8	-0.206588000	-0.454016000	0.000010000
1	1.628054000	-0.218170000	-0.894281000
1	1.009701000	1.221978000	-0.000575000
1	1.627683000	-0.217232000	0.894848000
6	-1.198858000	0.389206000	0.000007000
1	-2.079492000	-0.300291000	-0.000056000



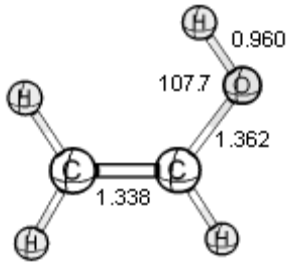
4′

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.081431000	0.160108000	-0.000001000
8	0.205446000	-0.503569000	-0.000003000
1	-1.619284000	-0.160739000	-0.894321000
1	-1.618900000	-0.159964000	0.894830000
1	-0.931044000	1.244236000	-0.000493000
6	1.326560000	0.149475000	0.000004000
1	1.054885000	1.247521000	-0.000010000



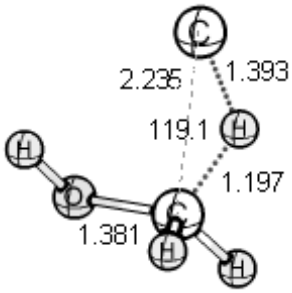
6

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.172178000	-0.147392000	-0.000009000
6	-0.236976000	0.401097000	-0.000049000
8	-1.233305000	-0.278861000	0.000011000
1	1.707620000	0.218437000	0.884575000
1	1.149447000	-1.239306000	-0.000741000
1	1.708292000	0.219697000	-0.883652000
1	-0.310130000	1.509830000	0.000084000



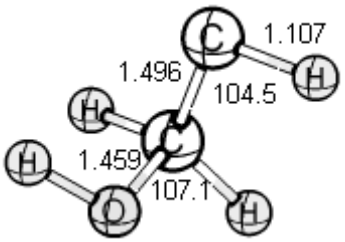
13

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.032563000	0.442810000	-0.000003000
8	1.209048000	-0.118121000	-0.000018000
6	-1.203096000	-0.205148000	-0.000010000
1	0.034449000	1.526709000	0.000039000
1	-1.261852000	-1.291055000	-0.000058000
1	1.099061000	-1.071525000	0.000170000
1	-2.130088000	0.354863000	0.000074000



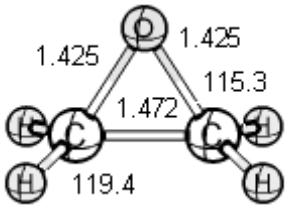
15

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.757004000	-0.297513000	-0.021149000
8	1.037499000	-0.492394000	-0.084283000
6	0.267447000	0.645905000	0.052830000
1	0.625197000	-1.168683000	0.458928000
1	-0.796192000	0.594304000	-0.493510000
1	0.100402000	0.983694000	1.078567000
1	0.707946000	1.439488000	-0.559810000



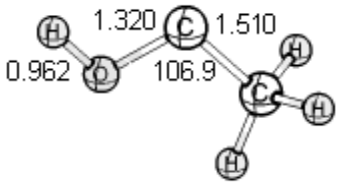
16a

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-1.308421000	-0.712149000	0.841511000
6	-0.089599000	0.730970000	-0.008546000
8	0.849530000	-0.377140000	0.131428000
6	-1.008969000	-0.435325000	-0.187904000
1	0.129022000	1.354319000	-0.877879000
1	1.024686000	-0.703088000	-0.756259000
1	-0.050116000	1.304166000	0.919907000



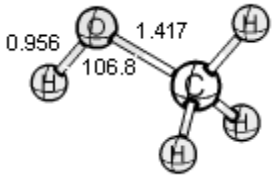
17

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-1.269826457	-0.645070409	-0.921945809
6	0.735735227	-0.423079439	0.000000334
8	0.000036877	0.797388286	-0.000000693
6	-0.735778773	-0.423036987	-0.000000643
1	1.269785570	-0.645202017	0.921932150
1	-1.269830427	-0.645070862	0.921948191
1	1.269804540	-0.645220564	-0.921919850



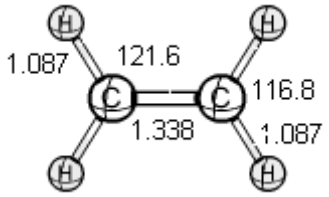
19

Atomic Number	X	Y	Z
8	1.100922000	0.282119000	0.000000000
6	0.137395000	-0.619553000	-0.000001000
6	-1.170171000	0.136226000	-0.000001000
1	1.933305000	-0.199837000	-0.000001000
1	-1.741742000	-0.192876000	-0.877131000
1	-1.060587000	1.228533000	-0.000037000
1	-1.741693000	-0.192818000	0.877183000



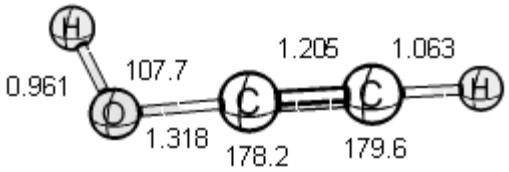
Methanol

Atomic Number	X	Y	Z
6	-0.046899000	0.659601000	0.000000000
8	-0.046899000	-0.757167000	0.000000000
1	-1.091639000	0.979761000	0.000000000
1	0.439751000	1.076887000	0.893225000
1	0.439751000	1.076887000	-0.893225000
1	0.868719000	-1.033799000	0.000000000



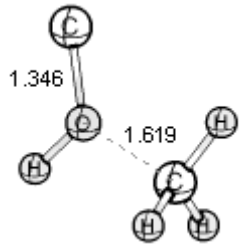
Ethylene

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000000	0.000000000	0.668919000
6	0.000000000	0.000000000	-0.668919000
1	0.000000000	0.925721000	-1.238825000
1	0.000000000	-0.925721000	-1.238825000
1	0.000000000	-0.925721000	1.238825000
1	0.000000000	0.925721000	1.238825000



CHCOH

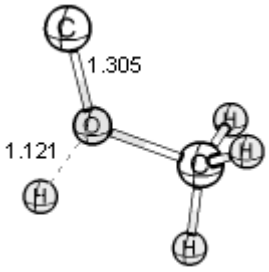
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000000	0.123891000	0.000000000
6	0.233711000	1.306485000	0.000000000
8	-0.295718000	-1.160438000	0.000000000
1	0.432340000	2.351178000	0.000000000
1	0.531139000	-1.649929000	0.000000000



1/2

Im. Freq. (cm^{-1})= -706.2950

Atomic Number	X	Y	Z
6	-1.209192000	-0.177900000	-0.000027000
8	0.320559000	0.351430000	0.000095000
1	-1.030751000	-1.250579000	-0.001777000
1	-1.669711000	0.199263000	0.914535000
1	0.319620000	1.324450000	-0.000284000
1	-1.671124000	0.202134000	-0.912740000
6	1.457107000	-0.369885000	-0.000054000



1/3

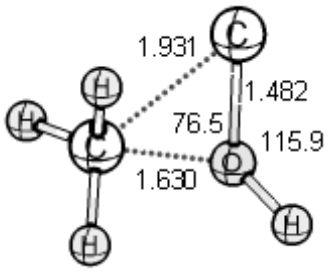
Im. Freq.(cm^{-1})= -1549.0497

Atomic Number	X	Y	Z
6	-1.092242000	-0.196829000	-0.000249000
1	-1.737268000	0.691776000	-0.039946000
1	-1.208274000	-0.762263000	0.922091000
1	-1.179094000	-0.828543000	-0.881442000
8	0.283489000	0.349774000	-0.000580000
6	1.376312000	-0.363550000	0.000585000
1	0.152301000	1.463108000	0.001916000

1/4

Im. Freq.(cm^{-1})= -1348.6686

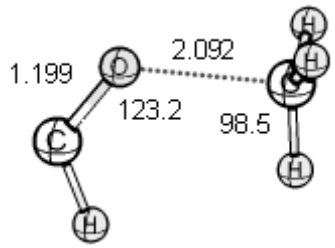
Atomic Number	X	Coordinates (Angstroms) Y	Z
6	-1.470162000	0.392576000	0.006740000
6	1.115714000	0.201207000	0.029190000
8	-0.163853000	-0.470997000	-0.122943000
1	1.021076000	1.113621000	-0.562868000
1	1.281986000	0.444733000	1.079887000
1	-0.760359000	-0.887008000	0.595920000
1	1.894807000	-0.466067000	-0.344976000



1’/19

Im. Freq.(cm^{-1})= -1182.1452

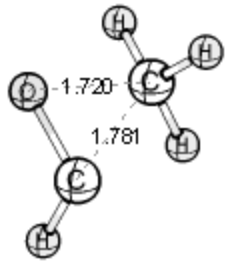
Atomic Number	X	Coordinates (Angstroms) Y	Z
6	-0.806920000	0.838411000	-0.022965000
8	-0.498552000	-0.602721000	0.128608000
6	0.971916000	0.088235000	-0.001858000
1	-0.791254000	-1.191541000	-0.619190000
1	1.405599000	0.232321000	0.979159000
1	0.963653000	0.969140000	-0.673271000
1	1.420439000	-0.748030000	-0.566624000



4/5

Im. Freq.(cm^{-1})= -397.4412

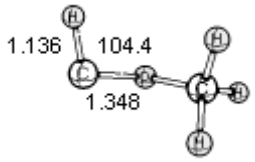
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.193358000	0.831901000	0.000000000
8	0.000000000	0.717485000	0.000000000
6	0.974206000	-1.133297000	0.000000000
1	-1.840971000	-0.082630000	0.000000000
1	1.527645000	-1.037699000	0.924109000
1	1.527645000	-1.037699000	-0.924109000
1	0.100593000	-1.773471000	0.000000000



4/6

Im. Freq.(cm^{-1})= -1006.0802

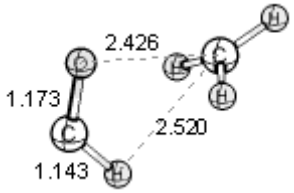
Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.556828000	-0.681817000	-0.025495000
6	0.704457000	0.596858000	0.192589000
1	1.128328000	1.088159000	-0.734563000
6	-0.987644000	0.075247000	-0.002845000
1	-1.333576000	-0.729394000	-0.658954000
1	-1.393283000	0.042746000	0.999492000
1	-1.156972000	1.020391000	-0.540486000



4/4′

Im. Freq.(cm^{-1})= -1063.3687

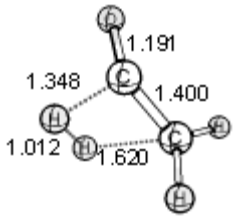
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.076736000	0.180633000	-0.008817000
8	0.171310000	-0.503703000	0.057997000
1	-1.197055000	0.665002000	-0.984763000
1	-1.846442000	-0.577995000	0.128343000
1	-1.154369000	0.932574000	0.788288000
6	1.279928000	0.220943000	-0.194547000
1	1.608239000	0.600580000	0.824335000



4′/11

Im. Freq.(cm^{-1})= -307.3105

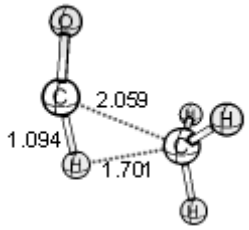
Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.781705000	-0.612450000	0.000000000
6	-1.555342000	0.038786000	0.000000000
6	1.226763000	0.472829000	0.000000000
1	-1.124118000	0.348756000	-0.938979000
1	-2.597165000	-0.271478000	0.000000000
1	-1.124118000	0.348756000	0.938979000
1	0.563234000	1.403880000	0.000000000



6/8

Im. Freq.(cm^{-1})= -1822.7559

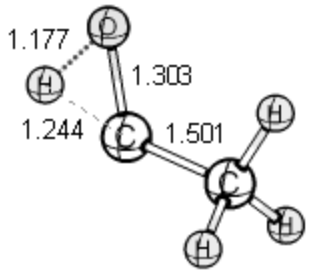
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.182893000	-0.224648000	0.031844000
6	-0.150423000	0.179575000	-0.108977000
8	-1.273258000	-0.195867000	0.019084000
1	0.600811000	1.157602000	0.643810000
1	1.432857000	-1.275738000	0.168538000
1	1.927880000	0.440284000	-0.391615000
1	0.029705000	1.515222000	-0.110611000



6/11

Im. Freq.(cm^{-1})= -1845.7965

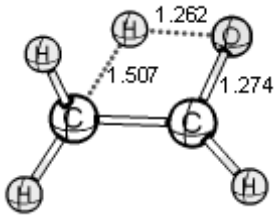
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.379019000	-0.144095000	0.000000000
6	-0.551785000	0.571461000	0.000000000
8	-1.278940000	-0.345796000	0.000000000
1	2.261875000	0.506625000	-0.000003000
1	1.332688000	-0.754151000	0.906054000
1	1.332684000	-0.754155000	-0.906051000
1	0.340874000	1.203851000	0.000000000



6/19

Im. Freq.(cm^{-1})= -2202.2363

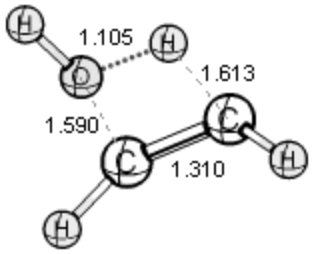
Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1.028583000	1.234793000	0.000000000
6	-1.105472000	-0.480373000	0.000000000
6	0.000000000	0.534330000	0.000000000
8	1.218823000	0.072887000	0.000000000
1	-1.735145000	-0.325394000	0.883624000
1	-0.676049000	-1.490845000	0.000000000
1	-1.735145000	-0.325394000	-0.883624000



13/6

Im. Freq.(cm^{-1})= -2409.2859

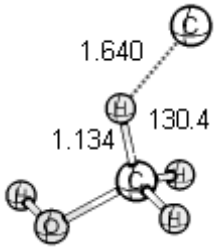
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.117842000	0.534969000	0.045047000
8	-1.098873000	-0.275484000	-0.021490000
6	1.108227000	-0.184850000	-0.052051000
1	-0.320751000	1.606050000	0.131930000
1	1.284419000	-0.772917000	0.852338000
1	-0.120755000	-1.014644000	-0.320557000
1	2.005762000	0.284671000	-0.449760000



13/14

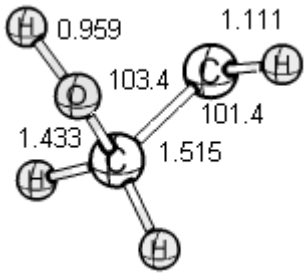
Im. Freq.(cm-1)= -1241.0954

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-2.209049000	-0.239636000	0.044057000
6	-0.280776000	0.589382000	0.001465000
8	1.110477000	-0.173172000	-0.102187000
6	-1.134081000	-0.403884000	0.020616000
1	-0.090331000	1.653629000	-0.034579000
1	1.539526000	-0.153275000	0.764738000
1	0.365179000	-0.988330000	-0.089205000



15/16a

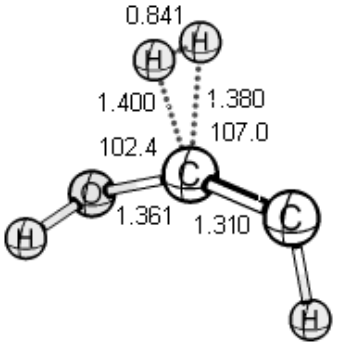
Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.628938000	-0.382510000	-0.048163000
6	-0.184652000	0.401106000	0.055951000
8	-1.425284000	-0.230648000	-0.127843000
6	2.261319000	-0.228667000	-0.028537000
1	-0.076226000	0.884385000	1.034045000
1	-1.552318000	-0.831854000	0.606911000
1	-0.058130000	1.140529000	-0.734534000



16a/16b

Im. Freq.(cm^{-1})= -468.0055

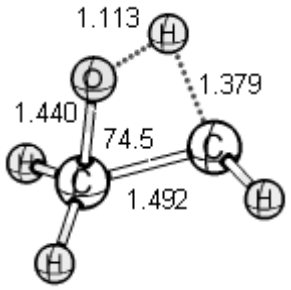
Atomic Number	X	Coordinates (Angstroms) Y	Z
1	-1.211903000	-0.942554000	0.763133000
6	-0.082443000	0.594626000	0.016039000
8	1.029985000	-0.306121000	0.093843000
6	-1.269564000	-0.329530000	-0.161683000
1	0.050858000	1.303160000	-0.809727000
1	1.156164000	-0.657462000	-0.789622000
1	-0.122960000	1.155245000	0.959338000



16a/27

Im. Freq.(cm^{-1})= -1356.1659

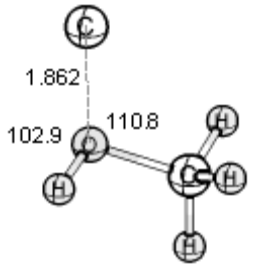
Atomic Number	X	Coordinates (Angstroms) Y	Z
1	1.569249000	-1.202272000	-0.064999000
6	0.128497000	0.182793000	-0.006834000
8	-1.172108000	-0.204022000	-0.109829000
6	1.402661000	-0.121420000	0.019100000
1	0.016174000	1.490898000	0.479478000
1	-1.433849000	-0.538655000	0.751303000
1	0.038342000	1.513965000	-0.360746000



16b/17

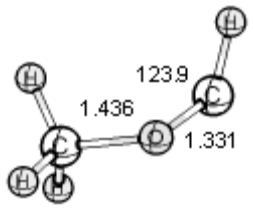
Im. Freq.(cm^{-1})= -1354.6286

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-1.447869000	-0.284502000	0.848815000
6	0.206520000	0.738927000	-0.017076000
8	0.674469000	-0.619078000	0.087505000
6	-1.010504000	-0.114274000	-0.144894000
1	0.577580000	1.266282000	-0.895405000
1	-0.092827000	-1.035740000	-0.603355000
1	0.391270000	1.258669000	0.921725000



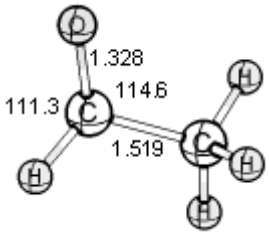
1T

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.654601000	-0.373444000	0.025844000
6	-1.070588000	-0.310523000	0.024277000
8	0.055201000	0.567616000	-0.131735000
1	-1.032932000	-1.001982000	-0.816979000
1	-0.999205000	-0.871528000	0.960741000
1	0.083434000	1.165492000	0.620357000
1	-1.996984000	0.270892000	-0.010960000



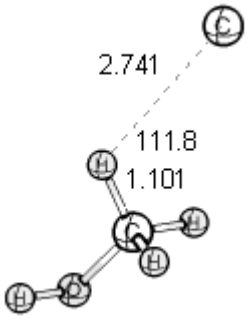
4T

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.079803000	0.195166000	-0.000692000
8	-0.162603000	-0.523077000	-0.047221000
1	1.224690000	0.641628000	0.988022000
1	1.864980000	-0.536357000	-0.198877000
1	1.095458000	0.978786000	-0.766649000
6	-1.249098000	0.216017000	0.165571000
1	-1.868532000	0.633459000	-0.634005000



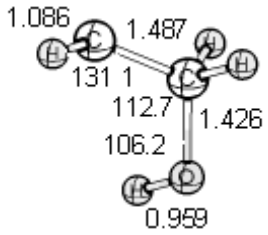
6T

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.157294000	-0.162061000	0.019123000
6	0.199890000	0.498873000	-0.145393000
8	1.235455000	-0.313624000	0.029265000
1	-1.937354000	0.563562000	-0.226149000
1	-1.247571000	-1.015626000	-0.659782000
1	-1.310443000	-0.519633000	1.047232000
1	0.356153000	1.459817000	0.362202000



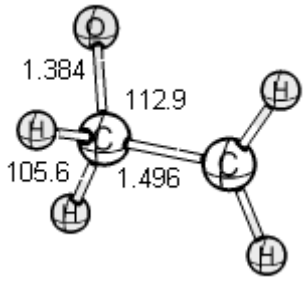
15T

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.549712000	1.465528000	0.109265000
6	0.383922000	0.386076000	-0.015466000
8	1.595465000	-0.342783000	-0.089456000
6	-2.877570000	-0.182586000	0.019061000
1	-0.260920000	0.035544000	0.804578000
1	2.049976000	-0.210028000	0.742039000
1	-0.140595000	0.230279000	-0.961807000



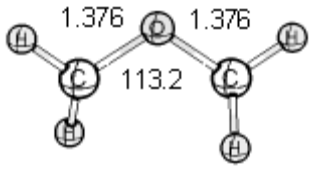
16T

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-1.761864000	-0.974432000	0.549541000
6	-0.052645000	0.538565000	0.000128000
8	1.107299000	-0.285859000	0.096895000
6	-1.307272000	-0.250086000	-0.120390000
1	0.023466000	1.240582000	-0.842950000
1	1.104577000	-0.843237000	-0.683100000
1	-0.065068000	1.133084000	0.922924000



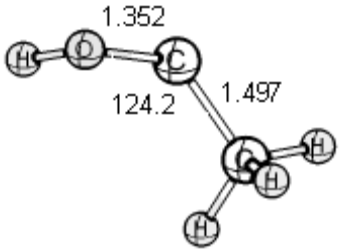
17T

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.190407000	-0.361257000	-0.087182000
6	-1.204930000	-0.222498000	-0.021402000
6	0.108205000	0.487645000	0.068350000
1	-1.303374000	-1.204023000	0.429135000
1	-2.065403000	0.247635000	-0.484714000
1	0.160800000	1.347673000	-0.617863000
1	0.265061000	0.907889000	1.089209000



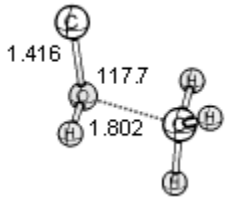
18T

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000000	1.148720000	-0.225139000
8	0.000000000	0.000000000	0.532072000
6	0.000000000	-1.148720000	-0.225139000
1	-0.029116000	2.046245000	0.381158000
1	0.559302000	1.121496000	-1.158613000
1	-0.559302000	-1.121496000	-1.158613000
1	0.029116000	-2.046245000	0.381158000



19T

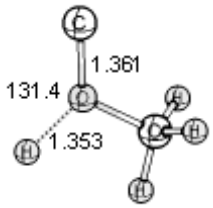
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.098172000	0.518698000	0.021285000
6	-1.253988000	-0.122828000	0.007620000
8	1.260470000	-0.157113000	-0.116266000
1	-2.028986000	0.646688000	0.061506000
1	-1.399438000	-0.700020000	-0.917047000
1	-1.384590000	-0.806689000	0.860805000
1	1.664155000	-0.258290000	0.751431000



1T/2

Im. Freq.(cm^{-1})= -1364.3879

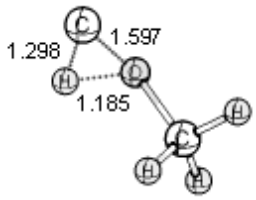
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.289997000	-0.188982000	0.021059000
8	0.385738000	0.453832000	-0.136927000
1	-1.270482000	-0.892777000	-0.804377000
1	-1.294752000	-0.640982000	1.010089000
1	0.407047000	1.077866000	0.605552000
1	-1.937996000	0.674175000	-0.116240000
6	1.458378000	-0.452508000	0.045673000



1T/3

Im. Freq.(cm^{-1})= -2601.2689

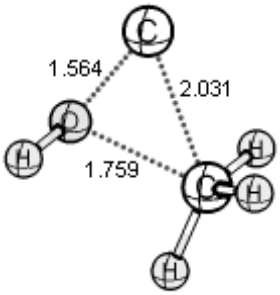
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.053374000	-0.226168000	0.000001000
1	1.754129000	0.611073000	-0.000227000
1	1.163657000	-0.833012000	-0.900476000
1	1.163819000	-0.832658000	0.900698000
8	-0.256217000	0.381003000	-0.000004000
6	-1.375532000	-0.393482000	0.000003000
1	-0.098923000	1.724475000	0.000015000



1T/4T

Im. Freq.(cm^{-1})= -1346.6098

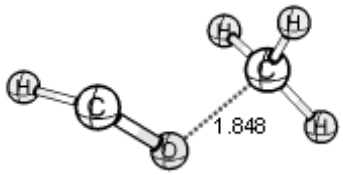
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.440141000	0.376116000	-0.050385000
6	1.079212000	0.216801000	0.016384000
8	-0.138443000	-0.548831000	-0.092063000
1	1.303989000	0.624061000	-0.971618000
1	0.948882000	1.034150000	0.731734000
1	-0.849069000	-0.362535000	0.837743000
1	1.869316000	-0.462530000	0.342653000



1T/19T

Im. Freq.(cm^{-1})= -1238.5887

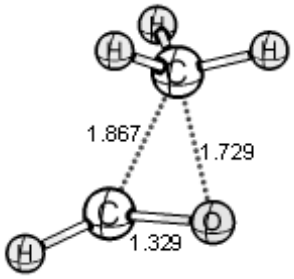
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.034302000	0.084122000	-0.009928000
8	0.561972000	-0.643818000	0.120675000
6	0.829713000	0.889945000	-0.024686000
1	-1.483696000	-0.899491000	-0.183870000
1	-1.255943000	0.462358000	0.981118000
1	-1.276083000	0.778760000	-0.810687000
1	0.747478000	-1.035479000	-0.744275000



4T/5

Im. Freq.(cm^{-1})= -957.3543

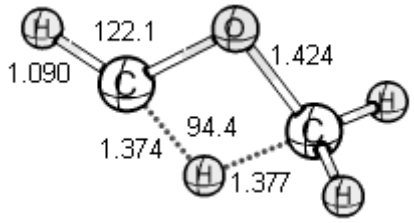
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.340329000	0.172496000	0.004457000
8	-0.372124000	-0.520477000	-0.059273000
1	1.390557000	0.592639000	1.005337000
1	1.932504000	-0.722198000	-0.161290000
1	1.339695000	0.892617000	-0.810215000
6	-1.311015000	0.255253000	0.168547000
1	-1.861646000	0.834264000	-0.597678000



4T/6T

Im. Freq.(cm^{-1})= -1418.3065

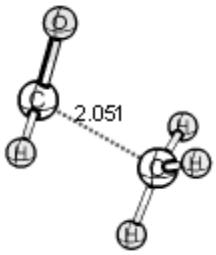
Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.477406000	0.734405000	0.023441000
6	0.808550000	-0.539941000	-0.154553000
1	1.414442000	-1.129613000	0.543864000
6	-1.008841000	-0.148894000	0.017671000
1	-1.559430000	0.791906000	-0.098489000
1	-1.279159000	-0.814438000	-0.806234000
1	-1.193347000	-0.590084000	0.994624000



4T/18T

Im. Freq.(cm^{-1})= -2252.5272

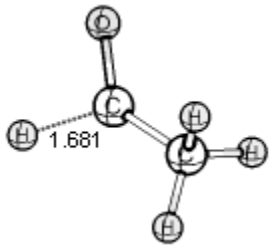
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.991380000	-0.224429000	-0.019602000
8	-0.115583000	0.670749000	0.015414000
6	-1.021814000	-0.356304000	0.061675000
1	1.599943000	-0.122427000	-0.918352000
1	1.519710000	-0.309544000	0.929611000
1	0.038480000	-1.213759000	-0.109203000
1	-2.050872000	-0.235863000	-0.277808000



6T/5

Im. Freq.(cm^{-1})= -543.1638

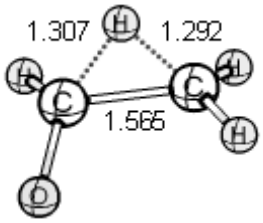
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.406400000	-0.146920000	0.010762000
6	0.512498000	0.550318000	-0.185238000
8	1.235384000	-0.388379000	0.051189000
1	-1.972909000	0.747240000	-0.236842000
1	-1.393056000	-0.930230000	-0.740712000
1	-1.445632000	-0.478189000	1.045169000
1	0.291934000	1.347829000	0.569734000



6T/7

Im. Freq.(cm^{-1})= -1258.7764

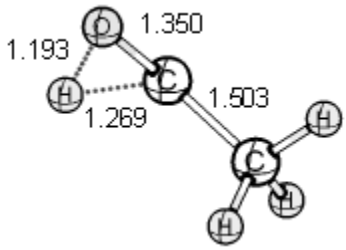
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.188116000	-0.124524000	0.057349000
6	0.249291000	0.261509000	-0.347029000
8	1.246410000	-0.231249000	0.109917000
1	-1.891165000	0.662513000	-0.217194000
1	-1.424004000	-1.031024000	-0.510073000
1	-1.245950000	-0.340848000	1.129247000
1	0.222782000	1.737439000	0.456764000



6T/17T

Im. Freq.(cm^{-1})= -1990.3751

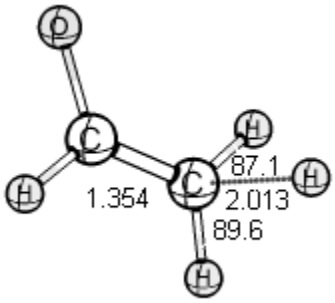
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.166594000	-0.209863000	-0.022634000
8	-1.160109000	-0.343309000	-0.066754000
6	-0.210646000	0.524237000	0.098101000
1	0.721833000	0.427645000	1.009128000
1	1.132046000	-1.275236000	0.169985000
1	1.899650000	0.206859000	-0.705271000
1	-0.208345000	1.500962000	-0.392610000



6T/19T

Im. Freq.(cm^{-1})= -2170.1007

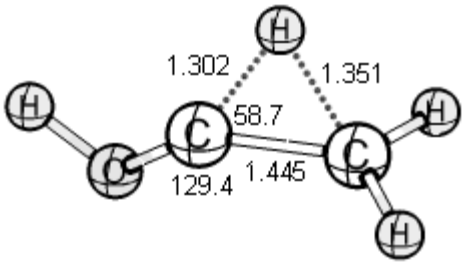
Atomic Number	X	Y	Z
6	-1.243254000	-0.106463000	0.035419000
8	1.297717000	-0.238081000	-0.010583000
6	0.141432000	0.437264000	-0.181162000
1	-1.462534000	-0.852469000	-0.739453000
1	-1.338188000	-0.585754000	1.019304000
1	-1.975609000	0.700981000	-0.042711000
1	1.005532000	0.657081000	0.721984000



6T/20

Im. Freq.(cm^{-1})= -809.4916

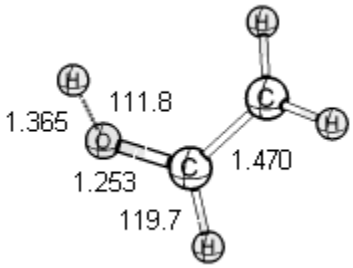
Atomic Number	X	Y	Z
6	-1.089103000	-0.073093000	-0.209957000
6	0.151371000	0.409215000	0.041204000
8	1.280709000	-0.278997000	-0.000044000
1	-1.913894000	0.625685000	-0.260913000
1	-1.224422000	-1.071346000	-0.609853000
1	-1.813082000	-0.781010000	1.529290000
1	0.332125000	1.441915000	0.354344000



13T/19T

Im. Freq.(cm^{-1})= -2195.5977

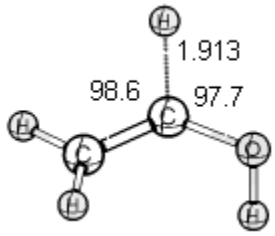
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.293559000	-0.138396000	-0.001391000
6	0.045700000	0.395427000	-0.102433000
1	-1.549187000	-0.746607000	0.867520000
8	1.247630000	-0.253317000	-0.029064000
1	1.899203000	0.392060000	0.253212000
1	-0.874209000	1.001334000	0.591448000
1	-1.969691000	-0.162432000	-0.856722000



13T/20

Im. Freq.(cm^{-1})= -2282.6310

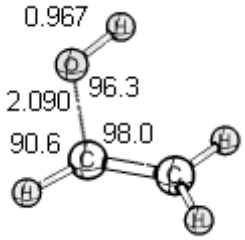
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.227062000	-0.200322000	-0.004302000
6	0.070446000	0.490770000	-0.030845000
1	-2.096304000	0.275446000	0.438902000
8	1.144283000	-0.153699000	-0.076429000
1	1.133049000	-1.220277000	0.775367000
1	0.093726000	1.574588000	0.135792000
1	-1.345043000	-1.142852000	-0.527743000



13T/21

Im. Freq.(cm^{-1})= -1121.5471

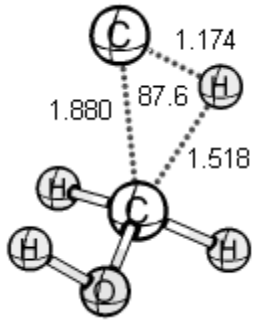
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.013887000	0.303381000	-0.297907000
8	1.216471000	-0.092335000	0.042797000
6	-1.223276000	-0.208085000	0.031376000
1	-0.075207000	1.891808000	0.766724000
1	-2.106709000	0.097754000	-0.516588000
1	1.230280000	-1.054642000	0.048136000
1	-1.357153000	-0.768012000	0.958539000



13T/24

Im. Freq.(cm^{-1})= -506.2182

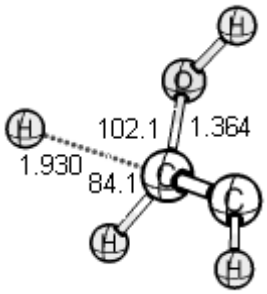
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.436796000	0.724549000	-0.196325000
8	1.439989000	-0.152292000	0.081442000
6	-1.187225000	-0.356958000	0.054904000
1	-0.126313000	1.593206000	0.367176000
1	-1.540925000	-1.004845000	-0.744938000
1	1.291685000	-0.907448000	-0.504606000
1	-1.400233000	-0.668122000	1.079358000



15T/16T

Im. Freq.(cm^{-1})= -765.5837

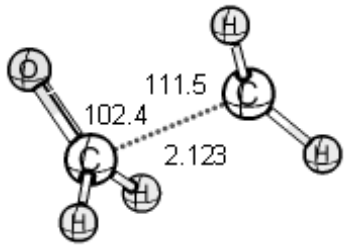
Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1.141155000	0.408582000	-0.764812000
6	-0.100597000	0.598152000	0.087827000
8	-1.061981000	-0.349345000	-0.098784000
6	1.488472000	-0.403338000	0.008258000
1	0.135966000	0.878883000	1.118734000
1	-0.784852000	-1.125298000	0.400495000
1	-0.323667000	1.463709000	-0.540659000



16T/22

Im. Freq.(cm^{-1})= -877.8054

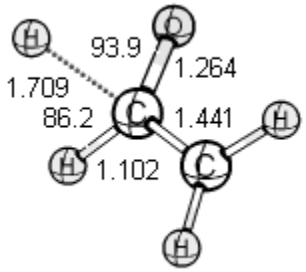
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.218207000	-0.384697000	0.052308000
8	1.176350000	-0.151565000	-0.008871000
6	-0.092574000	0.311473000	-0.197741000
1	-2.275292000	-0.177799000	-0.017158000
1	-0.284622000	1.570136000	1.253342000
1	1.113595000	-0.943013000	0.531127000
1	-0.099793000	1.202539000	-0.823744000



17T/10T

Im. Freq.(cm^{-1})= -489.4942

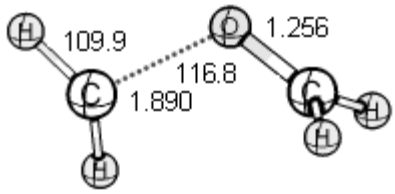
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.490603000	0.547953000	0.067850000
8	1.159773000	-0.478386000	-0.067572000
1	0.292875000	0.975391000	1.066964000
1	0.302966000	1.226716000	-0.783620000
6	-1.498246000	-0.184693000	-0.057011000
1	-2.231244000	0.595365000	-0.231057000
1	-1.596929000	-1.149948000	0.423252000



17T/20

Im. Freq.(cm^{-1})= -1099.6941

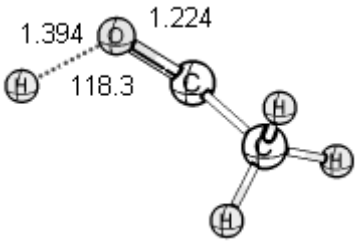
Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.152191000	-0.349580000	-0.025657000
6	-1.195926000	-0.197677000	0.010208000
6	0.120060000	0.373985000	-0.124666000
1	-1.289593000	-1.208402000	0.392656000
1	-2.085048000	0.380138000	-0.220781000
1	0.190777000	1.358259000	-0.615420000
1	0.421533000	1.208792000	1.335554000



18T/10T

Im. Freq.(cm^{-1})= -847.5473

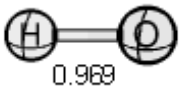
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.225990000	0.221365000	0.035436000
8	-0.246533000	-0.558701000	-0.066998000
1	-1.699669000	0.648791000	-0.857890000
1	-1.580104000	0.558087000	1.018073000
6	1.473009000	0.212895000	0.067776000
1	1.544210000	1.222658000	-0.325676000
1	2.225709000	-0.565489000	0.082207000



19T/7

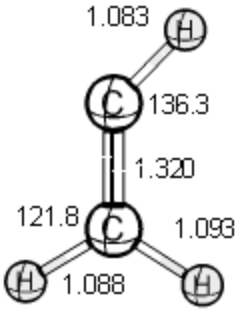
Im. Freq.(cm^{-1})= -2097.4689

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.133664000	-0.445083000	-0.203348000
6	-1.247878000	0.119789000	0.029305000
8	1.193520000	0.028962000	0.185182000
1	-2.012356000	-0.634422000	-0.165003000
1	-1.335769000	0.495311000	1.055621000
1	-1.390667000	0.956781000	-0.668351000
1	1.875916000	0.902390000	-0.659457000



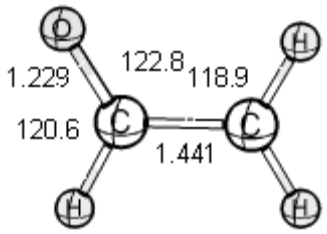
Singlet OH radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.000000000	0.000000000	0.107692000
1	0.000000000	0.000000000	-0.861534000



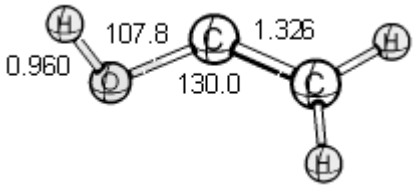
Doublet CH_2CH radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.050319000	-0.591615000	0.000000000
6	0.050319000	0.727906000	0.000000000
1	-0.881459000	-1.163714000	0.000000000
1	0.975174000	-1.165410000	0.000000000
1	-0.697549000	1.511375000	0.000000000



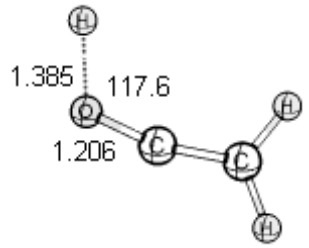
Doublet CH_2-CHO radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.054737000	-0.548006000	0.000000000
6	0.000000000	0.433375000	0.000000000
8	-1.191233000	0.130838000	0.000000000
1	2.099337000	-0.252391000	0.000000000
1	0.791421000	-1.601012000	0.000000000
1	0.310687000	1.494483000	0.000000000



Doublet CH_2-COH radical

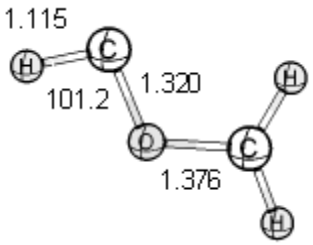
Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.027224000	-0.418843000	-0.019522000
8	1.171108000	0.181358000	-0.080095000
6	-1.243288000	0.108717000	0.020143000
1	-2.119418000	-0.523230000	-0.055949000
1	1.747522000	-0.250994000	0.554551000
1	-1.373892000	1.184121000	0.138433000



TS CH_2-COH/CH_2-CO + H

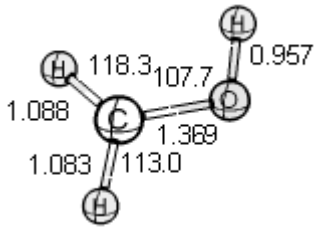
Im. Freq.(cm^{-1})= -2054.2230

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000000	0.183361000	0.000000000
8	-1.203454000	0.101870000	0.000000000
6	1.291710000	-0.065107000	0.000000000
1	1.625739000	-1.099942000	0.000000000
1	-1.760732000	-1.165805000	0.000000000
1	2.012363000	0.741256000	0.000000000



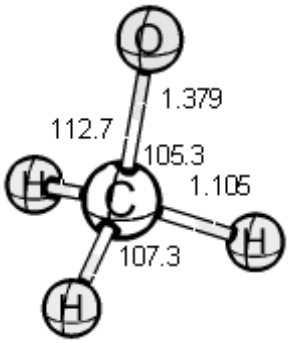
Doublet CH_2O-CH radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.123755000	0.157390000	-0.029800000
1	-1.949043000	-0.524193000	0.112660000
1	-1.147601000	1.236447000	0.046976000
6	1.154112000	0.371940000	0.007480000
8	0.114469000	-0.441450000	-0.004787000
1	1.998747000	-0.356634000	0.012580000



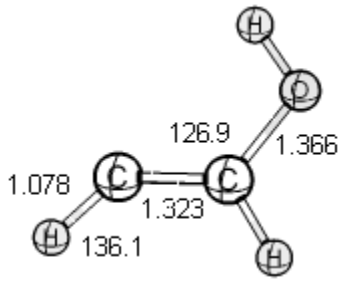
Doublet CH_2OH radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.683972000	0.027744000	-0.076644000
8	-0.672462000	-0.124515000	0.028601000
1	1.228577000	-0.889796000	0.111012000
1	1.119812000	0.982344000	0.210171000
1	-1.072524000	0.737111000	-0.090127000



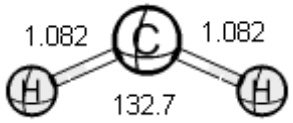
Doublet CH_3O radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.009134000	0.797204000	0.000000000
6	0.009134000	-0.582033000	0.000000000
1	-1.056657000	-0.872840000	0.000000000
1	0.464389000	-1.006298000	0.906293000
1	0.464389000	-1.006298000	-0.906293000



Doublet CH-CHOH radical

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.108911000	0.390289000	-0.000408000
8	1.166013000	-0.099906000	0.000135000
6	-1.229653000	-0.312228000	-0.000032000
1	-0.110489000	1.480646000	0.000760000
1	-2.285292000	-0.091785000	0.000758000
1	1.099060000	-1.057975000	0.000049000



Triplet methylene

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000000	0.000000000	0.108650000
1	0.000000000	0.991415000	-0.325951000
1	0.000000000	-0.991415000	-0.325951000