Exploration of the potential energy surface of C4H4 for rearrangement and decomposition reactions of vinylacetylene : A computational study

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Supporting Information

Table S1. Energies, enthalpies, entropies, and dipole moments of structures **1 - 43**, dissociation products **DP1 - DP9**, and transition states for reactions **R1- R30** located at the PES of C_4H_4. [a]

♯	Mole-cule	State	Sym.	Method	ΔE (A)	ΔE (B)	ZPE (B)	$\Delta\Delta H(298)$ (A)	$\Delta\Delta H(298)$ (B)	low. freq. (B)	μ (B)	S (B)	$\Delta H_f^o(298)$ (B)	$\Delta H_f^o(298)$ CCSD(T) (C)	Ref.
1	**1**	$^1A'$	C_s	RDFT	-154.74043	-154.79540	38.3	-154.67390	-154.72900	226	0.42	66.2	70.4*		main Ref
2				RMP2	-154.23682	-154.38933	38.5	-154.16985	(-154.32249)	219	0.51	66.9			
3				GVB-MP2	-154.25389		(38.5)	(-154.18692)							
4				CASSCF(6,6)	-153.81153		(38.3)	(-153.74500)			0.34				
5	**2**	^1A_g	D_{2h}	RDFT	2.1	3.4	37.6	1.8	2.9	225	0	63.7			83.0*
6				RMP2	11.8	11.5	38.3	11.8	11.5	227	0	64.0	81.9		2, RMP2/B
7	**3**	$^1A_1$	C_{2v}	RDFT	20.2	22.4	38.0	19.8	21.9	361	2.13	63.0	92.3	94.0	1
8	**4**	$^1A'$	C_s	RDFT	A*	36.1	37.9	A*	35.8	45	3.84	69.0	106.2	106.6	1; 102.5*
9	**5**	^1A_g	D_{2h}	RDFT		A*	38.3	A*	38.8	534	0	63.2	109.2	103.8	1
10	**6**	$^1A'$	C_s	RDFT	A*	47.4	36.7	A*	46.1	139	2.79	68.4	116.5	116.4	1
11	**7**	^1A	C_1	RDFT	A*	47.4	38.7	A*	47.3	519	1.98	62.6	115.1	113.9	1
12	**8**	$^1A'$	C_s	RDFT	A*	49.4	37.5	A*	49.0	144	5.45	69.2	119.4	120.7	1
13	**9**	$^1A'$	C_s	RDFT	A*	54.5	38.6	A*	54.3	438	3.74	62.3	124.7	121.4	1
14	**10**	$^1A'$	C_s	RDFT	A*	57.1	35.6	A*	55.2	82	3.64	71.7	125.6	130.8	1
15	**11**	$^1A'$	C_s	RDFT	→ **10**										
16	**12**	$^1A'$	C_s	BSDFT	A*	56.3	37.8	A*	55.3	520	2.68	62.7	125.7	125.7	1
17	**13**	$^1A'$	C_s	RDFT	A*	56.6	38.3	A*	56.7	142	4.39	66.3	127.1	124.3	1
18	**14a**	$^3A''$	C_s	RODFT	62.0	64.1	35.9	60.0	62.0	207	0.82	69.7			
19				UDFT	58.8	61.0	35.9	56.8	58.8	207	0.76	69.9	129.2 [0]	134.6	1
20				UMP2	77.2	79.8	38.7	77.3	(79.9)	221	0.45	68.5			
21	TS	$^1A'$	C_s	BSDFT	62.9	63.9	35.8	60.2	(61.8)	302i	2.84	65.8			
22		^1A	C_1	BSDFT	62.4	63.4	35.9	60.2	61.3	163	2.86	67.8	131.7 [2.5]		1
23	**14b**	$^3A''$	C_s	RODFT	62.4	64.3	35.7	60.1	61.9	216	0.75	69.7			
24				UDFT	59.1	61.0	35.6	56.8	58.6	206	0.74	69.9	129.0 [-0.2]	134.7	1
25				UMP2	78.1	80.9	38.3	77.8	(80.6)	244	0.67	68.5			
26	TS	$^1A'$	C_s	BSDFT	64.2	(65.0)	35.4	61.2	(62.6)	155i	2.33	65.9			
27		^1A	C_1	BSDFT	64.1	64.9	35.4	61.7	62.4	158	2.52	68.5	132.8 [3.6]		1
28	**15**	$^1A_1$	T_d	RDFT	A*	63.3	37.3	A*	61.9	571	0	62.7	132.3	130.9	1
29	**16**	$^1A'$	C_s	BSDFT	70.8	72.3	35.4	68.5	69.8	106	1.36	68.8	140.2 [11.0]	144.9	1
30				GVB-MP2	74.0		(35.4)	(71.7)			1.25	(68.8)	142.1 [13.1]		3, GVB-MP2/A
31	**17**	$^1A'$	C_s	BSDFT	71.4	73.1	35.5	69.2	70.7	112	0.41	70.0	141.4 [11.9]	145.7	1
32				GVB-MP2	→ **3**										
33	**18**, TS	$^1A'$	C_s	BSDFT	72.8	74.5	35.1	69.7	71.3	223i	0.77	66.8	141.7 [12.5]		1
34				GVB-MP2	74.4		(35.3)	(71.3)			1.02	(66.8)	141.7 [12.5]		3, GVB-MP2/A
35	**19**	$^1A'$	C_s	BSDFT	→ **3**										
36				GVB-MP2	62.8		(35.4)	(59.9)			0.68	(68.4)	133.2 [4.0]		3, GVB-MP2/A
37	**20**	$^1A_1$	C_{2v}	RDFT	A*	71.4	38.8	A*	71.6	366	0.84	63.2	142.0	137.2	1
38	**21**	^1A_g	C_{2h}	BSDFT	72.4	74.0	36.2	70.4	71.9	144	0	66.1	142.3 [13.1]	146.3	1
39	**22**	$^1A_1$	C_{2h}	BSDFT	A*	74.8	35.8	A*	72.4	180	0	65.5	142.8	146.9	1
40	**23**	$^1A\prime$	C_s	BSDFT	A*	75.2	35.8	A*	72.9	163	1.17	67.1	143.3	147.4	1
41	**24**	$^1A_1$	C_{2v}	BSDFT	A*	77.8	35.6	A*	75.4	108	1.12	67.1	145.8	149.9	1
42	**25**	^1A	C_2	BSDFT	76.0	77.4	35.6	73.8	74.8	108	0.13	67.4	145.2 [16.0]	148.8	1
43	**26**, TS	$^1A\prime$	C_s	BSDFT	A*	78.1	35.5	A*	75.2	77i	1.00	65.3	145.6	149.5	1
44	**27a**	^1A	C_1	RDFT	A*	83.1	36.5	A*	81.5	145	2.43	67.8	151.9	1 50.5	1
45	**27b**	^1A	C_1	RDFT	A*	83.2	35.2	A*	80.4	196	2.43	68.0	150.8	150.0	1
46	**28**	^1A	C_1	R → U	68.2	70.9	36.2	66.4	69.0	130	2.89	67.6	139.4 [47.1]	141. 4	1
47	**29**	^1A	C_1	R → U	90.6	91.3	35.8	88.1	88.8	190	3.76	66.2	159.2 [66.9]	161.0	1
48	**30**	$^1A'$	C_s	BSDFT	A*	87.6	37.2	A*	86.4	332	2.14	65.0	156.8	159.2	1
49	**31**,TS	$^1A'$	C_s	UDFT	→ **TS(8,8′)**										
50	**32**	^1A	C_1	BSDFT	A*	100.5	35.0	A*	97.7	163	4.65	69.8	168.1	171.9	1
51	**33**	^1A	C_1	BSDFT	A*	68.6	37.4	A*	67.4	414	1.37	63.7	137.8	141.7	1
52	**34**,TS	$^1A'$	C_s	U/RDFT	→ **TS(7,7′)**										
53	**35**	$^1A_1$	C_{2v}	RDFT	→ **TS(20,20′)**										
54	**36**	$^1A'$	C_s	RDFT	→ **13**										
55	**37**	$^1A'$	C_s	U/RRDFT	→ **3**										
56	**38**	$^1A'$	C_s	BSDFT	A*	117.5	34.9	A*	114.6	141	3.16	70.1	185.0	188.5	1
57	**39**	$^1A'$	C_s	U/RRDFT	→ **6**										
58	**40**	$^1A_1$	C_{2v}	BSDFT	102.0	103.6	33.5	97.6	99.3	601i	2.14	68.4	169.7	171.1	1
59	**41**	$^1A'$	C_s	BSDFT	A*	128.7	33.6	A*	124.7	119	4.44	71.1	195.1	197.4	1
60	**42**	$^1A'$	C_s	RRDFT	→ **4**										
61	**43**	^1A	C_1	RRDFT	→ **9**										
62	**DP1**	$(^1\text{ß}_g^+,^1\text{ß}_g^+)$	$(D_{\infty h},D_{\infty h})$	RDFT	47.9	45.6	30.0	41.8	39.3			89.8	109.7	111.6	102*
63	**DP2a**	$^1A_1$	C_{2v}	RDFT	49.3	43.6	34.2	46.6	41.1	31	0.32	82.7	111.5	109.9	1
64	**DP2**	$^1A_1$	C_{2v}	RDFT	51.0	44.4	33.8	47.6	41.2			95.6	111.6	110.7	108.7*

65	**DP3**	$^1A_1$	C_{2v}	RDFT	A*	87.1	28.7		80.0	162	4.62	95.4	150.4	155.6	1
66	**DP4**	($^1\mathrm{B}_g^+$, $^1A_1$)	($D\infty h$, C_{2v})	RDFT	92.6	87.7	31.7	87.6	82.7			100.9	153.1	153.2	154.6*
67	**DP5**	$^1A'$	C_s	RDFT	→ **DP1**										
68	**DP6**	$^1A_1$	C_{2v}	RDFT	A*	102.3	28.4	A*	94.4	105	0.10	97.0	164.8	172.7	1
69	**DP7**	$^1A'$	C_s	RDFT	→ **DP6**										
70	**DP8a**	$^1A'$	C_s	RDFT	A*	118.3	29.6	A*	111.1	214	0.37	94.8	181.6	184.6	1
71	**DP8b**	$^1A'$	C_s	RDFT	A*	118.3	29.4	A*	111.0	224	0.83	94.7	181.4	183.1	1
72	**DP9**	($^1A_1$, $^1A_1$)	(C_{2v}, C_{2v})	RDFT	134.1	130.9	29.6	127.5	124.2	344	2.51	106.3	203.2	195.7	200.3*
73	**TS(1,2)**	^1A	C_1	RDFT	A*	94.1	34.1	A*	89.9	780i	3.65	66.4	160.3	161.2	1
74	**TS(1,3)**	^1A	C_1	BSDFT	A*	99.9	33.1	A*	94.5	2098i	0.56	64.7	164.9	162.8	1
75	**TS(1,4)**	^1A	C_1	RDFT	A*	99.7	3481	A*	96.0	1283i	3.96	64.6	166.4	169.3	1
76	**TS(1,5)**	^1A	C_1	RDFT	A*	99.0	34.9	A*	95.4	1012i	1.82	65.2	165.8	158.7	1
77	**TS(1,6)**	$^1A'$	C_s	RDFT	A*	47.5	36.0	A*	45.2	157i	3.03	65.8	115.6	114.7	1
78	**TS(1,10)**	^1A	C_1	RDFT	A*	71.4	34.6	A*	67.8	1189i	2.24	66.5	138.2	140.8	1
79	**TS(1,14b)**	^1A	C_1	RDFT	A*	84.6	33.6	A*	80.1	798i	3.57	66.6	150.5	156.5	1
80	**TS(1,22)**	$^1A'$	C_s	BSDFT	A*	97.6	33.0	A*	92.3	1806i	0.30	65.7	162.7	159.2	1
81	**TS(1,27a)**	^1A	C_1	RDFT	A*	83.1	35.2	A*	80.0	334i	1.70	66.6	150.4	149.5	1
82	**TS(1,27b)**	^1A	C_1	RDFT	A*	83.3	34.7	A*	79.4	303i	2.59	66.0	149.8	149.6	1
83	**TS(1,33)**	^1A	C_1	BSDFT	A*	92.8	35.2	A*	89.6	871i	1.75	65.2	160.0	158.5	1
84	**TS(1,DP4)**	$^1A'$	C_s	RDFT	109.0	108.0	32.7	104.0	103.3	1244i	1.53	71.0	173.7	173.4	1
85	**TS(1,DP5)** anti	$^1A'$	C_s	RDFT	101.7	102.4	30.7	95.1	95.8	389i	1.77	68.5	166.2	168.1	1
86	**TS(1,DP5)** syn	$^1A'$	C_s	RDFT	A*	100.2	31.1	A*	93.4	389i	1.74	68.6	163.8	165.7	1
87	**TS(2,13)**	^1A	C_1	RDFT	A*	72.2	37.1	A*	70.7	301i	3.91	63.7	141.1	139.7	1
88	**TS(2,28)**	^1A	C_1	RDFT	A*	71.3	36.2	A*	68.9	253i	3.06	64.7	139.3	140.7	1
89	**TS(2,DP1)**	$^1A_1$	C_{2v}	RDFT	95.8	95.0	31.5	89.0	88.1	1477i	0.97	64.9	158.5	160.5	1
90	**TS(2,DP3)**	^1A	C_1	RDFT	97.0	96.7	31.2	90.3	90.0	748i	2.12	68.0	160.4	167.7	1
91	**TS(3,14b)**	^1A	C_1	BSDFT	66.9	64.9	35.9	64.2	64.6	217i	2.58	65.1	135.0	139.0	1
92	**TS(3,29)**	^1A	C_1	BSDFT	A*	104.1	34.3	A*	99.9	700i	2.72	64.3	170.3	171.5	1
93	**TS(3,DP2)**	^1A	C_1	RDFT	A*	114.7	32.4	A*	109.4	1068i	6.05	71.8	179.8	184.6	1
94	**TS(3,DP4)**	^1A	C_1	RDFT	A*	89.3	34.0	A*	85.6	248i	1.99	71.1	156.0	156.2	1
95	**TS(4,6)**	^1A	C_1	RDFT	A*	98.8	35.0	A*	95.3	1271i	4.00	65.0	165.7	168.1	1
96	**TS(5,3)**	^1A	C_1	RDFT	A*	119.7	33.3	A*	114.7	653i	4.97	66.3	185.1	192.6	1
97	**TS(6,3)**	$^1A'$	C_s	RDFT	67.4	69.1	35.4	64.2	65.9	580i	1.78	64.0	136.3	136.2	1
98	**TS(7,7′)**	$^1A'$	C_s	RDFT	A*	66.6	37.9	A*	65.5	560i	3.45	61.9	135.9	133.6	1
99	**TS(7,9)**	^1A	C_1	RDFT	A*	110.0	35.0	A*	106.4	1511i	2.96	63.2	176.8	171.9	1
100	**TS(7,12)**	^1A	C_1	RDFT	106.1	109.3	34.6	102.1	105.2	1552i	1.73	62.8	175.6	173.2	1
101	**TS(7,13)**	^1A	C_1	RDFT	A*	106.7	35.6	A*	103.7	1309i	2.38	63.3	174.1	169.1	1
102	**TS(8,8′)**	^1A	C_1	RDFT	A*	94.9	36.1	A*	92.8	602i	3.79	66.8	163.2	161.3	1
103	**TS(9,15)**	$^1A'$	C_s	RDFT	A*	99.0	35.2	A*	95.3	1048i	2.64	62.1	165.7	162.0	1
104	**TS(10,4)**	^1A	C_1	RDFT	A*	98.9	35.6	A*	96.4	995i	2.10	68.4	166.8	167.4	1
105	**TS(10,DP1)**	^1A	C_1	RDFT	A*	104.4	31.5	A*	98.1	1505i	2.63	68.5	168.5	177.3	1
106	**TS(12,5)**	$^1A_1$	C_{2v}	BSDFT	A*	66.6	38.1	A*	66.0	732i	1.39	62.0	136.4	139.4	1
107	**TS(12,15)**	$^1A'$	C_s	BSDFT	A*	93.5	35.9	A*	90.6	708i	1.17	62.6	161.0	155.5	1
108	**TS(13,13′)**	$^1A_1$	C_{2v}	RDFT	A*	57.1	37.9	A*	56.3	56i	4.34	62.5	126.7	123.8	1
109	**TS(14b,2)**	^1A	C_1	RDFT	79.0	78.9	34.2	75.0	74.9	452i	2.01	66.7	145.3	150.9	1
110	**TS(20,20′)**	^1A_g	D_{2h}	RDFT	A*	81.11	38.3	A*	80.4	383i	0	59.0	150.8	146.2	1
111	**TS(20,28)**	^1A	C_1	RDFT	A*	94.1	34.1	A*	89.9	780i	3.65	66.4	160.3	146.9	1
112	**TS(22,24)**	^1A	C_1	BS-DFT	A*	80.9	35.1	A*	77.5	168i	0.80	63.9	147.9	147.9	1
113	**TS(22,DP2)**	$^1A'$	C_s	BSDFT	A*	80.8	33.8	A*	76.8	880i	0.20	68.4	147.2	144.2	1
114	**TS(24,5)**	$^1A'$	C_s	BSDFT	A*	80.4	35.5	A*	77.4	342i	0.81	65.1	147.8	145.0	1
115	**TS(27a,27b)**	^1A	C_1	RDFT	A*	87.8	35.5	A*	85.0	407i	2.05	66.2	155.4	153. 6	1
116	**TS(27a,DP1)**	^1A	C_1	RDFT	A*	115.1	32.1	A*	109.0	1349i	2.70	67.0	144.4	184.2	1
117	**TS(27a,DP2)**	^1A	C_1	RDFT	A*	118.5	33.1	A*	113.4	1226i	3.77	67.1	183.8	187.5	1
118	**TS(27b,DP1)**	^1A	C_1	RDFT	A*	114.2	31.7	A*	107.8	1528i	3.36	66.9	178.2	181.9	1
119	**TS(27b,DP2)**	^1A	C_1	RDFT	A*	120.3	33.0	A*	115.1	975i	3.34	66.8	185.5	190.1	1
120	**TS(28,3)**	^1A	C_1	RDFT	A*	88.5	35.0	A*	84.9	933i	2.61	64.4	155.3	155.7	1
121	**TS(29,12)**	^1A	C_1	RDFT	A*	93.1	36.3	A*	90.7	186i	4.14	63.3	161.1	160.2	1
122	**TS(29,DP2)**	^1A	C_1	RDFT	A*	95.3	34.8	A*	91.9	482i	4.16	66.3	162.3	164.4	1
123	**TS(DP3,DP1)**	$^1A'$	C_s	RDFT	A*	157.5	25.2	A*	146.2	1637i	2.79	94.8	216.6	214.6	1
124	**TS(DP4,DP2)**	^1A	C_1	RDFT	A*	91.5	30.1	A*	84.8	853i	3.15	100.9	155.2	154.4	1
125	**TS(DP5,DP1)**	$^1A'$	C_s	RDFT	→ DP1										

[a] Absolute energies (enthalpies) in hartree, relative energies (enthalpies) in kcal/mol, lowest frequency (low. freq.) in cm^{-1}, dipole moment μ in Debye, entropies S in cal mol/deg. Each calculation has a number, which is given in the first column. Values in parentheses were derived using ZPE and temperature corrections from basis A calculations. Accordingly, lowest frequency and entropy are also from basis A calculations. In many cases, preliminary calculations were carried out with the 6-31+G(d) basis or done directly with basis B, which is indicated by A* in the columns that contain A results. - Values in brackets give energies of excited states relative to the corresponding ground state energy. For each state, the most reliable energy obtained was used to calculate $\Delta H_f^0(298)$ values. In addition, the $\Delta H_f^0(298)$ values obtained at the CCSD(T)/basis C level of theory (Tables S2 and S3) are listed. The last column gives the number of the number of the reference calculation to clarify how $\Delta H_f^0(298)$ value was obtained using basis B. Experimental heats of formation are indicated by a star. Basis A: 6-31G(d,p); basis B: 6-311++G(3df,3pd); basis C: Dunning's cc-pVTZ [4s,3p,2d1f/3s,2p1d] The following notation was used: *BSDFT*: a stability test was made and, in case of instability, the calculation was carried out at the BS-UDFT level of theory; *U/RDFT*: The calculation was started with BS-UDFT and switched to RDFT after some cycles; the relative energies of columns 6 and 7 were calculated with regard to the reference given in the last cloumn via the line number ♯.

Table S2. CCSD(T)/cc-pVTZ and G2M energies E, zero-point corrected energies E_0, and enthalpies ΔH(298) of minimum structures encountered on the C_4H_4 PES. [a)]

Molecule	E CCSD(T)	E_0 CCSD(T)	H(298) CCSD(T)	ΔE CCSD(T)	ΔE_0 CCSD(T)	ΔΔH(298) CCSD(T)	ΔE_0 G2M	ΔΔH(298) G2M
1	-154.443874	-154.382887	-154.377469	0.0	0.0	0.0	0.0	0.0
2	-154.430753	-154.370784	-154.365123	8.2	11.0	7.7	7.4	7.6
3	-154.405377	-154.344487	-154.339850	24.1	23.9	23.6	23.5	23.2
4	-154.385860	-154.325466	-154.319839	36.1	36.0	36.2	35.2	35.4
5	-154.389918	-154.328886	-154.324165	33.8	33.8	33.4	33.7	33.2
6	-154.368600	-154.310059	-154.304214	47.2	45.7	46.0	46.0	46.3
7	-154.374431	-154.312743	-154.308173	43.6	44.0	43.5	43.2	42.7
8	-154.362956	-154.303197	-154.297241	50.8	50.0	50.3	50.1	50.4
9	-154.362357	-154.300721	-154.296221	51.0	51.6	51.0	50.8	50.2
10	-154.344635	-154.287790	-154.281209	62.3	59.7	60.4	55.8	56.7
11	-> **10**							
12	-154.357209	-154.297006	-154.289366	55.3	53.9	55.3	52.6	52.1
13	-154.358119	-154.296827	-154.291502	53.8	54.0	53.9	54.0	53.9
14a	-154.330158	-154.272984	-154.267240	71.4	69.0	69.2	68.9	69.1
14b	-154.327839	-154.271400	-154.265468	72.8	70.0	70.3	69.7	70.0
15	-154.345342	-154.285868	-154.281113	61.8	60.9	60.5	59.2	58.8
16	-154.321226	-154.264777	-154.258766	77.0	74.1	74.5	74.2	74.6
17	-154.320146	-154.263593	-154.257441	77.6	74.9	75.3	74.9	75.3
18	-> **3**							
19	-> **3**							
20	-154.337695	-154.275790	-154.271012	66.6	67.2	66.8	65.9	65.5
21	-154.319517	-154.256519	-154.256519	78.0	75.7	75.9	76.6	76.8
22	-154.318202	-154.255499	-154.255499	78.9	76.4	76.5	77.3	77.4
23	-154.317583	-154.254805	-154.354805	79.3	76.8	77.0	77.7	77.9
24	-154.313323	-154.250819	-154.250819	81.9	79.2	79.5	80.1	80.4
25	-154.315023	-154.252491	-154.252491	80.9	78.2	78.4	78.9	79.1
26	-154.313056	-154.251360	-154.251360	82.1	79.3	79.1	80.3	80.1
27a	-154.313611	-154.249795	-154.249795	81.7	79.9	80.1	80.5	80.6
27b	-154.312663	-154.250620	-154.250620	82.3	79.3	79.6	80.1	80.4
28	-154.327757	-154.264320	-154.264320	72.9	70.8	71.0	70.5	70.7
29	-154.295482	-154.233041	-154.233041	93.1	90.6	90.6	90.0	90.1
30	-154.300399	-154.241050	-154.235949	90.0	89.0	88.8	86.6	86.4
31	-154.294673	-154.237133	-154.231682	93.6	91.5	91.5	90.8	90.9
32	-154.277693	-154.221963	-154.215761	104.3	101.1	101.5	100.5	101.1
33	-154.328218	-154.268635	-154.263766	72.6	71.7	71.3	69.1	68.7
35	-> **TS(20,20')**							
36	-> **13**							
37	-> **3**							
38	-154.251073	-154.195458	-154.189199	121.0	117.6	118.1	118.1	118.8
39	-> **6**							
40	-> **TS(28,28')**							
41	-154.234986	-154.181450	-154.175047	131.1	126.4	127.0	126.5	127.1
42	-> **4**							
43	-> **9**							
DP1	-153.195736	-153.157929	-153.152741	47.6	39.3	41.2	38.4	40.4
DP2	-77.187301	-77.160473	-77.156614	43.5	38.9	40.3	38.9	40.2
DP2a	-154.376876	-154.322380	-154.314479	42.0	38.0	39.5	37.8	39.3
DP3	-153.123994	-153.088340	-153.082729	92.6	83.0	85.2	82.4	84.6
DP4	-77.1167091	-77.093125	-77.088871	87.8	81.1	82.8	81.4	83.0
DP5	-> **DP1**							

DP6	-153.768510	-153.723164	-153.716960	110.2	100.4	102.3	103.6	105.6
DP7	-> **DP6**							
DP8a	-153.753073	-153.705855	-153.698075	119.9	111.2	114.2	114.1	115.6
DP8b	-153.752852	-153.705927	-153.700469	120.0	111.2	112.7	114.1	115.6
DP9	-154.233418	-154.320946	-154.313228	132.1	123.4	125.3	123.9	125.8
H	-0.499810	-0.499810	-0.497450				-0.50000	-0.497640
H_2	-1.172337	-1.162290	-1.158986				-1.16664	-1.163338

[a)] Absolute values in Hartree, relative values in kcal/mol. CCSD(T) and G2M calculations used a BS-UHF wave function in those cases, in which BS-UDFT was necessary to appropriately describe biradicaloid structure (see Table S1). E_0 and ΔH(298) values were calculated using the thermochemistry of B3LYP/6-311++G(3df,3pd) level of theory. For the numbering of structures, see Scheme 2. For H and H_2 absolute CCSD(T) and G2M values are given to calculate the relative energies of some of the DP structures.

Table S3. CCSD(T)/cc-pVTZ and G2M energies E, zero-point corrected energies E_0, and enthalpies ΔΔH(298). [a]

Structure	E CCSD(T)	E_0 CCSD(T)	H(298) CCSD(T)	ΔE CCSD(T)	ΔE_0 CCSD(T)	ΔΔH(298) CCSD(T)	ΔE_0 G2M	ΔΔH(298) G2M
TS(1,2)	-154.292570	-154.238153	-154.232720	94.9	90.8	90.8	90.2	90.2
TS(1,3) R	-154.288055	-154.235255	-154.230220	97.8	92.6	92.4		
TS(1,3) BS	-154.280631	-154.227830	-154.222796	102.4	97.3	97.1	98.2	97.9
TS(1,4)	-154.280353	-154.224850	-154.219800	102.6	99.2	98.9	97.9	97.6
TS(1,5)	-154.297512	-154.241919	-154.236728	91.8	88.5	88.3	88.2	88.1
TS(1,6)	-154.368582	-154.311144	-154.305863	47.2	45.0	44.9	45.1	45.0
TS(1,9)	-154.338259	-154.278876	-154.274297	66.3	65.3	64.7	64.6	64.0
TS(1,10)	-154.326007	-154.270824	-154.265319	74.0	70.3	70.4	70.3	70.3
TS(1,14b)	-154.299388	-154.245876	-154.240189	90.7	86.0	86.1	84.8	85.0
TS(1,22) R	-154.294118	-154.241491	-154.236146	94.0	88.7	88.7		
TS(1,22) BS	-154.279941	-154.227314	-154.221969	102.9	97.6	97.6	98.7	98.7
TS(1,27a)	-154.312915	-154.256853	-154.251435	82.2	79.1	79.1	80.0	80.0
TS(1,27b)	-154.311940	-154.256609	-154.251267	82.8	79.2	79.2	79.2	79.1
TS(1,33) R	-154.298444	-154.242340	-154.237132	91.3	88.2	88.1		
TS(1,33) BS	-154.290817	-154.230078	-154.225360	96.0	95.9	95.4	94.0	93.9
TS(1,DP4)	-154.271846	-154.219676	-154.213383	107.9	102.4	103.0	102.6	103.2
TS(1,DP5,syn)	-154.281279	-154.231680	-154.225592	102.0	94.9	95.3	94.8	95.2
TS(2,13)	-154.331048	-154.271857	-154.267084	70.8	69.7	69.3	68.8	68.4
TS(2,28)	-154.328050	-154.270399	-154.265392	72.7	70.6	70.3	70.0	69.7
TS(2,DP1)	-154.289234	-154.238978	-154.233832	97.0	90.3	90.1	89.8	89.6
TS(2,DP3)	-154.278060	-154.228364	-154.222338	104.1	97.0	97.3	96.5	96.8
TS(3,14b) R	-154.329598	-154.273385	-154.268105	71.7	68.7	68.6		
TS(3,14b) BS	-154.329126	-154.272912	-154.267632	72.0	69.0	68.9	68.4	68.4
TS(3,29) R	-154.276009	-154.221338	-154.216388	105.3	101.4	101.1		
TS(3,29) BS	-154.274604	-154.219932	-154.214982	106.2	102.3	102.0	101.9	101.6
TS(3,DP2)	-154.253473	-154.201855	-154.195490	119.5	113.6	114.2	111.2	111.8
TS(3,DP4)	-154.301234	-154.247108	-154.240806	89.5	85.2	85.8	85.5	86.0
TS(4,6)	-154.282671	-154.226943	-154.221835	101.2	97.9	97.7	97.1	96.9
TS(5,3)	-154.241199	-154.188185	-154.182742	127.2	122.2	122.2	120.9	120.9
TS(6,3)	-154.333917	-154.277454	-154.272593	69.0	66.2	65.8	66.0	65.6
TS(7,7')	-154.341425	-154.281017	-154.276732	64.3	63.9	63.2	64.4	63.7
TS(7,9)	-154.276289	-154.220473	-154.215723	105.2	101.9	101.5	101.2	100.7
TS(7,12)	-154.273360	-154.218268	-154.213604	107.0	103.3	102.8	102.2	101.8
TS(7,13)	-154.281729	-154.224906	-154.220134	101.7	99.1	98.7	98.4	98.0
TS(8,8')	-154.294673	-154.237133	-154.231682	93.6	91.5	91.5	90.8	90.9
TS(9,15)	-154.292069	-154.236011	-154.231481	95.3	92.2	91.6	91.0	90.5
TS(10,4)	-154.285365	-154.228702	-154.222938	99.5	96.8	97.0	95.0	95.2
TS(10,DP1)	-154.263459	-154.213250	-154.207092	113.2	106.4	106.9	105.8	106.3
TS(12,5)	-154.332893	-154.272155	-154.267437	69.6	69.5	69.0	67.8	67.4
TS(12,15) R	-154.303608	-154.246433	-154.241824	88.0	85.6	85.1		
TS(12,15) BS	-154.293647	-154.236472	-154.231863	94.3	91.9	91.4	91.0	90.4
TS(13,13')	-154.354276	-154.293834	-154.289114	56.2	55.9	55.4	55.8	55.3
TS(14b,2)	-154.309206	-154.254766	-154.249141	84.5	80.4	80.5	80.1	80.2
TS(20,28)	-154.320044	-154.260284	-154.255587	77.7	76.9	76.5	76.1	75.7
TS(22,24) R	-154.314952	-154.259054	-154.253898	80.9	77.7	77.5		
TS(22,24) BS	-154.310164	-154.254267	-154.249111	83.9	80.7	80.5	81.2	81.1
TS(22,DP2) R	-154.319901	-154.266029	-154.259936	77.8	73.3	73.8		
TS(22,DP2) BS	-154.307553	-154.253681	-154.247589	85.5	81.1	81.5	82.0	82.4
TS(24,5) R	-154.320213	-154.263571	-154.258511	77.6	74.9	74.6		
TS(24,5) BS	-154.309979	-154.253337	-154.248277	84.0	81.3	81.1	82.4	82.2
TS(27a27b)	-154.306865	-154.250239	-154.244914	86.0	83.2	83.2	82.5	82.5
TS(27a,DP1)	-154.252856	-154.201699	-154.196067	119.9	113.7	113.8	113.1	113.2
TS(27a,DP2)	-154.249306	-154.196552	-154.190925	122.1	116.9	117.1	115.8	116.0
TS(27b,DP1)	-154.255926	-154.205440	-154.199796	117.9	111.3	111.5	110.7	110.8
TS27b,DP2)	-154.244903	-154.192364	-154.186750	124.9	119.6	119.7	118.8	118.9
TS(28,3)	-154.302191	-154.246469	-154.241497	88.9	85.6	85.3	84.9	84.6
TS(28,28'), BS	-154.276514	-154.223157	-154.216975	105.0	100.2	100.7	100.2	100.8
TS(28,28'), R	-154.256917	-154.203560	-154.197378	117.3	112.5	113.0		
TS(29,12)	-154.296908	-154.239087	-154.234384	92.2	90.2	89.8	89.4	88.9
TS(29,DP2)	-154.288695	-154.233190	-154.227731	97.4	93.9	94.0	92.7	92.7

TS(33,9) R	-154.320490	-154.261632	-154.257112	77.4	76.1	75.5		
TS(33,9) BS	-154.316956	-154.258098	-154.253578	79.6	78.3	77.7	76.8	76.2
TS(DP3,DP1)	-154.196006	-154.155951	-154.147688	155.5	142.4	144.2	141.2	143.0
TS(DP4,DP2)	-154.299306	-154.251460	-154.243605	90.7	82.5	84.0	82.3	83.8

[a] Absolute values in Hartree, relative values in kcal/mol. CCSD(T) and G2M calculations used a BS-UHF wave function in those cases, in which BS-UDFT was necessary to appropriately describe biradicaloid structure (see Table S1). In some cases calculations were done with both a RHF and a BS-UHF wave function (indicated by R and BS after the structure symbol) to demonstrate the effect of the BS calculation. E_0 and DH(298) values were calculated using the thermochemistry of B3LYP/6-311++G(3df,3pd) level of theory. For the numbering of structures, see Scheme 3.

Figure S1

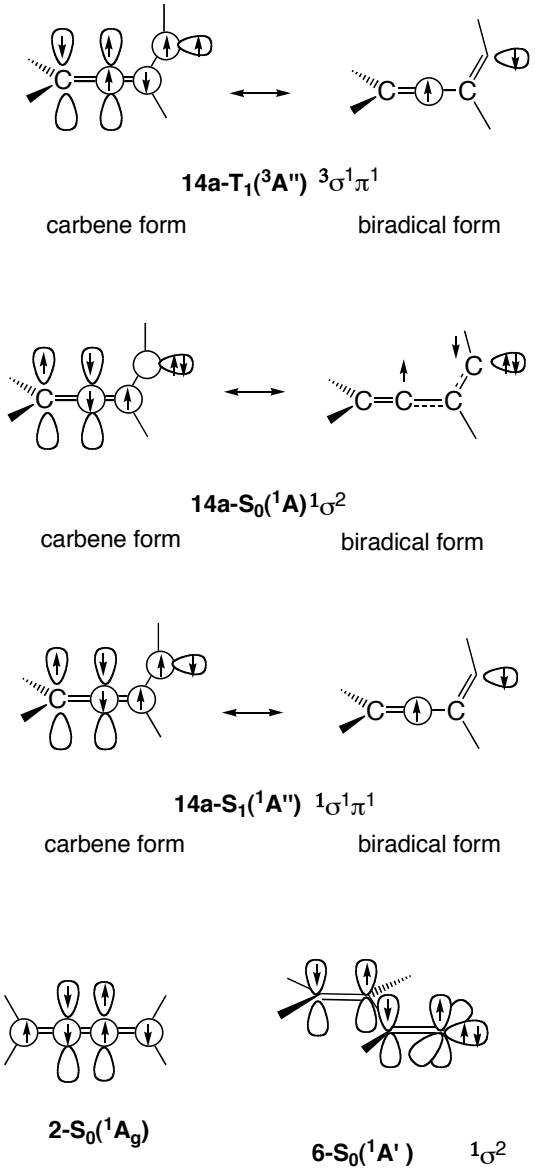


Figure S1. Explanation of the σ,π-notation used in the manuscript for the case of the three lowest states of carbene **14**, butatriene **2**, and carbene **6**. The electron configuration is given for each state considered.

Table S4:
Summary of equilibrium geometries of all calculated stationary points on the C4H4 PES

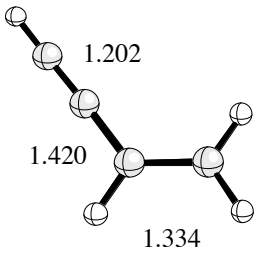
Calculations are done at the B3LYP/6-311++G(3df,3pd) level of theory if not noted otherwise.

In the following relevant data of a given structure are summarized in the order a) to g)
a) Number of structure (see Schemes 2 and 3)
b) Energies (method); convergent data, S**2 value
c) Frequencies
d) Thermochemical data
e) Equilibrium geometry in form of Cartesian coordinates given in the standard orientation
f) Rotational constants
g) Ball and Stick representation of the equilibrium geometry

1, Vinylacetylene (Reference)

E(RMP2) = -154.38933

```
SCF Done:  E(RB+HF-LYP) =  -154.795404862     A.U. after    8 cycles
             Convg  =    0.2961D-08             -V/T =  2.0051
             S**2   =   0.0000

1                     2                     3
                     A'                    A"                    A'
 Frequencies --   225.8140              320.9430              559.7856

Zero-point correction=                           0.060988 (Hartree/Particle)
 Sum of electronic and zero-point Energies=          -154.734417 (0)
 Sum of electronic and zero-point Energies=          -154.328342 (0)

 Sum of electronic and thermal Enthalpies=           -154.728999
 Sum of electronic and thermal Free Energies=        -154.760443

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  41.078             14.963             66.178

Dipole moment (field-independent basis, Debye):
    X=     0.0676    Y=    -0.4136    Z=     0.0000  Tot=     0.4191

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.119345   -1.692810    0.000000
    2          6             0        0.577404   -0.554895    0.000000
    3          6             0        0.000000    0.742478    0.000000
    4          6             0       -0.454499    1.855651    0.000000
    5          1             0       -0.867069    2.833262    0.000000
    6          1             0        1.661581   -0.591031    0.000000
    7          1             0        0.384385   -2.648804    0.000000
    8          1             0       -1.200260   -1.695977    0.000000
 ---------------------------------------------------------------------
Rotational constants (GHZ):     51.9653332      4.7492059      4.3515132
```



2

E(RMP2) =-154.3709692

SCF Done: E(RB+HF-LYP) = -154.789983471   A.U. after   5 cycles
             Convg =   0.2315E-08   -V/T = 2.0051
             S**2   =   0.0000

1	2	3
	B2U	B3U	B3G
Frequencies --	224.9164	229.1434	364.9605

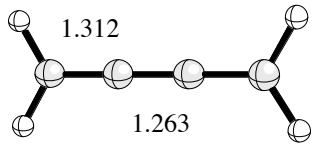
Zero-point correction=   0.059970 (Hartree/Particle)
Sum of electronic and zero-point Energies=   -154.730014 (2.8)
Sum of electronic and zero-point Energies=   -154.310999 (10.9)
Sum of electronic and thermal Energies=   -154.725295
Sum of electronic and thermal Enthalpies=   -154.724350
Sum of electronic and thermal Free Energies=   -154.754626

	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	40.593	15.298	63.720

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	1.942970
2	6	0.000000	0.000000	0.631456
3	6	0.000000	0.000000	-0.631456
4	6	0.000000	0.000000	-1.942970
5	1	0.000000	0.924452	-2.507766
6	1	0.000000	-0.924452	-2.507766
7	1	0.000000	-0.924452	2.507766
8	1	0.000000	0.924452	2.507766

Rotational constants (GHZ):   146.6909959   4.0261162   3.9185663



3

SCF Done: E(RB+HF-LYP) = -154.759640265   A.U. after   11 cycles
             Convg =   0.1012D-08   -V/T = 2.0051
             S**2   =   0.0000

1	2	3
	B2	B1	B1
Frequencies --	360.6181	429.0958	687.8781

 Sum of electronic and zero-point Energies=   -154.699110 (22.1)
 Sum of electronic and thermal Energies=   -154.695057
 Sum of electronic and thermal Enthalpies=   -154.694113 (21.9)
 Sum of electronic and thermal Free Energies=   -154.724049

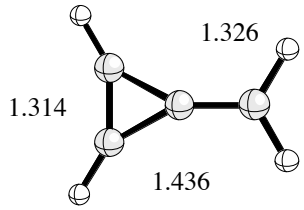
	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	40.526	13.984	63.005

 Dipole moment (field-independent basis, Debye):
    X=   0.0000   Y=   0.0000   Z=   -2.1345 Tot=   2.1345

Standard orientation:

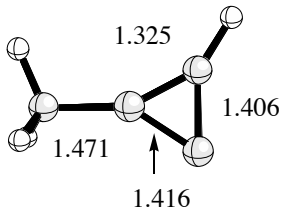
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.261011
2	6	0	0.000000	0.000000	1.587141
3	6	0	0.000000	0.656795	-1.016284

4	6	0	0.000000	-0.656795	-1.016284
5	1	0	0.000000	1.567107	-1.589618
6	1	0	0.000000	-1.567107	-1.589618
7	1	0	0.000000	0.926275	2.142865
8	1	0	0.000000	-0.926275	2.142865



4

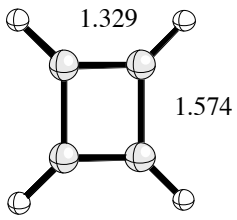
```
SCF Done:  E(RB+HF-LYP) =  -154.737898626     A.U. after    9 cycles
             Convg  =    0.2850D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --    45.2438              339.2772             386.1688

Zero-point correction=                           0.060393 (Hartree/Particle)
 Sum of electronic and zero-point Energies=          -154.677505 (35.7)
 Sum of electronic and thermal Energies=             -154.672822
 Sum of electronic and thermal Enthalpies=           -154.671878 (35.8)
 Sum of electronic and thermal Free Energies=        -154.704646

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.836             14.076            68.967

Dipole moment (field-independent basis, Debye):
    X=    -2.3252    Y=     3.0606    Z=     0.0014  Tot=     3.8437

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.147360    0.550105   -0.000015
    2          6             0       -0.052759   -0.011306    0.000022
    3          6             0        1.084815   -0.854851   -0.000023
    4          1             0        1.770595    1.429957    0.000001
    5          6             0       -1.522522    0.056074   -0.000113
    6          1             0       -1.903986   -0.467938    0.877929
    7          1             0       -1.903183    1.075633   -0.005350
    8          1             0       -1.904787   -0.477788   -0.871806
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     28.8277494      6.9020421      5.7647557
```



5

```
SCF Done:  E(UB+HF-LYP) =  -154.732904315     A.U. after   11 cycles
             Convg  =    0.2922D-08             -V/T =  2.0050
             S**2   =   0.0000
```

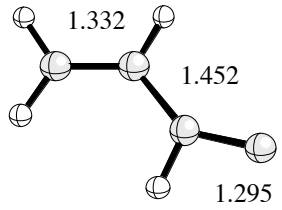
```
1                    2                    3
                    A"                   A"                   A"
 Frequencies --    534.2224             590.2118             604.9392

Zero-point correction=                          0.061032 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.671872 (39.2)
 Sum of electronic and thermal Energies=              -154.668095
 Sum of electronic and thermal Enthalpies=            -154.667151 (38.8)
 Sum of electronic and thermal Free Energies=         -154.697163

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.668             13.124            63.167

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.000

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.000060   -1.030194    0.000000
    2          1             0        0.092286   -2.105050    0.000000
    3          6             0       -1.015606   -0.172502    0.000000
    4          6             0        0.000000    1.030128    0.000000
    5          1             0       -0.092271    2.104991    0.000000
    6          6             0        1.015654    0.172579    0.000000
    7          1             0        2.090802    0.261387    0.000000
    8          1             0       -2.090741   -0.261391    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     17.1710440     12.8250512      7.3416062
```



6

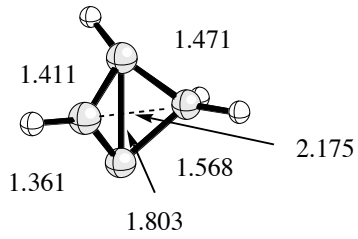
```
SCF Done:  E(RB+HF-LYP) =  -154.719843394     A.U. after    8 cycles
             Convg  =    0.2415D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                    A'                   A"                   A'
 Frequencies --    139.4514             176.8489             423.4395

Zero-point correction=                          0.058541 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.661302 (45.9)
 Sum of electronic and thermal Energies=              -154.656401
 Sum of electronic and thermal Enthalpies=            -154.655457 (46.1)
 Sum of electronic and thermal Free Energies=         -154.687946

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.811             15.408            68.381

Dipole moment (field-independent basis, Debye):
    X=     2.2031    Y=     1.7062    Z=     0.0000  Tot=     2.7866

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.249708    1.129096    0.000000
    2          6             0        0.000000    0.669063    0.000000
    3          6             0       -0.355531   -0.738771    0.000000
    4          6             0       -1.419691   -1.476049    0.000000
    5          1             0        0.432335   -1.516791    0.000000
    6          1             0        1.449201    2.190866    0.000000
    7          1             0        2.104579    0.466077    0.000000
```

```
    8          1             0       -0.833031    1.359818    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      54.1493589      4.8188299      4.4250392
```



7

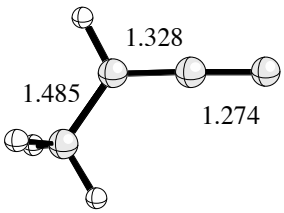
```
 SCF Done:  E(RB+HF-LYP) =  -154.719786629     A.U. after    7 cycles
              Convg  =    0.5249D-08             -V/T =  2.0050
              S**2   =    0.0000

1                     2                     3
                      A                     A                     A
 Frequencies --   519.3698              616.9781              656.1791

Zero-point correction=                           0.061687 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.658099 (47.9)
 Sum of electronic and thermal Energies=             -154.654473
 Sum of electronic and thermal Enthalpies=           -154.653529 (47.3)
 Sum of electronic and thermal Free Energies=        -154.683269

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.985             12.183            62.592

Dipole moment (field-independent basis, Debye):
    X=     0.0834    Y=     1.8205    Z=     0.7677  Tot=     1.9775

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.087874   -0.089480    0.139348
    2          6             0       -0.156998   -0.914573   -0.337701
    3          6             0       -1.086121   -0.061313    0.182077
    4          1             0       -2.155708   -0.021198    0.285419
    5          6             0       -0.030389    0.854032   -0.012410
    6          1             0       -0.033348    1.660788   -0.744082
    7          1             0        1.355801   -0.358364    1.151911
    8          1             0        1.947065   -0.013217   -0.521134
 ---------------------------------------------------------------------
```



8

```
SCF Done:  E(RB+HF-LYP) =  -154.716655264     A.U. after   12 cycles
             Convg  =    0.8745D-08             -V/T =  2.0050
             S**2   =    0.0000

1                     2                     3
                     A"                    A'                    A"
```

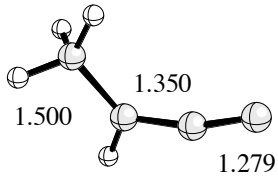
```
 Frequencies --   144.8100               190.5534               234.6601

Zero-point correction=                           0.059759 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.656896 (48.6)
 Sum of electronic and thermal Energies=             -154.651885
 Sum of electronic and thermal Enthalpies=           -154.650940 (49.0)
 Sum of electronic and thermal Free Energies=        -154.683820

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.644             15.089            69.200

Dipole moment (field-independent basis, Debye):
    X=    -3.6793    Y=     4.0229    Z=     0.0000  Tot=     5.4517

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.550359   -1.442295    0.000000
    2          6             0        0.790888   -0.419463    0.000000
    3          6             0        0.000000    0.647682    0.000000
    4          1             0        0.458704    1.636126    0.000000
    5          6             0       -1.484948    0.619572    0.000000
    6          1             0       -1.875901   -0.393127    0.000000
    7          1             0       -1.860299    1.162014    0.873035
    8          1             0       -1.860299    1.162014   -0.873035
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     41.8047127      4.7642444      4.3910147
```



8 triplet

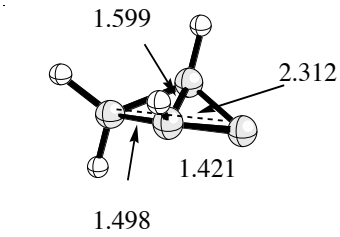
```
SCF Done:  E(UB+HF-LYP) =  -154.662291787     A.U. after    1 cycles
             Convg  =    0.2755D-08             -V/T =  2.0049
             S**2   =   2.0271

Dipole moment (field-independent basis, Debye):
    X=    -1.4787    Y=     2.3912    Z=     0.0000  Tot=     2.8114

1                    2                    3
                    A"                   A'                   A"
 Frequencies --    93.0022              206.6292              431.6108

Zero-point correction=                           0.057560 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.063465
Sum of electronic and zero-point Energies=           -154.604732 (81.4)
 Sum of electronic and thermal Energies=             -154.599771
 Sum of electronic and thermal Enthalpies=           -154.598827 (81.7)
 Sum of electronic and thermal Free Energies=        -154.632822

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.232             15.423            71.547

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.460280   -1.453686    0.000000
    2          6             0        0.900614   -0.303762    0.000000
    3          6             0        0.000000    0.701352    0.000000
    4          1             0        0.399444    1.711370    0.000000
    5          6             0       -1.489389    0.525113    0.000000
    6          1             0       -1.764388   -0.526405    0.000000
    7          1             0       -1.932043    1.000468    0.878901
```

```
   8          1             0       -1.932043    1.000468   -0.878901
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     33.7705401      4.9973532      4.4731576
```



9

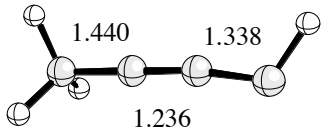
```
SCF Done:  E(RB+HF-LYP) =  -154.708560136     A.U. after   11 cycles
             Convg  =    0.9982D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A'                    A"                    A'
 Frequencies --   483.7195              728.1237              742.8108
Zero-point correction=                          0.061636 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.646924 (54.9)
 Sum of electronic and thermal Energies=             -154.643368
 Sum of electronic and thermal Enthalpies=           -154.642424 54.3)
 Sum of electronic and thermal Free Energies=        -154.672050

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.908             11.841            62.353

Dipole moment (field-independent basis, Debye):
    X=    -2.2436    Y=     3.0014    Z=     0.0000  Tot=     3.7472

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.610425   -1.119126    0.000000
    2          6             0       -0.104270    1.079967    0.000000
    3          6             0       -0.104270   -0.186753    0.799326
    4          6             0       -0.104270   -0.186753   -0.799326
    5          1             0        0.825601    1.632901    0.000000
    6          1             0       -0.989665    1.713602    0.000000
    7          1             0       -0.810817   -0.435256    1.583150
    8          1             0       -0.810817   -0.435256   -1.583150
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     19.6371763     11.5975127      8.6223267
```



10

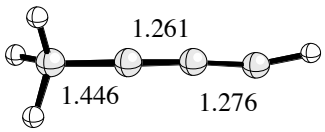
```
SCF Done:  E(RB+HF-LYP) =  -154.704400562     A.U. after   10 cycles
             Convg  =    0.4765D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                      A                     A                     A
 Frequencies --    81.8971              130.5136              188.7139

Zero-point correction=                          0.056845 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.647556 (54.5)
 Sum of electronic and thermal Energies=             -154.641918
 Sum of electronic and thermal Enthalpies=           -154.640974 (55.2)
 Sum of electronic and thermal Free Energies=        -154.675055
```

```
                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.208             16.728            71.729

Dipole moment (field-independent basis, Debye):
    X=     3.3561    Y=     1.4081    Z=     0.1231  Tot=     3.6416

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.861006    0.006559   -0.005326
    2          1             0        2.298850    0.914465   -0.425608
    3          1             0        2.283190   -0.871178   -0.500301
    4          1             0        2.175382   -0.044263    1.043293
    5          6             0        0.421268    0.010709   -0.015821
    6          6             0       -0.814624    0.013226   -0.003220
    7          6             0       -2.141694   -0.159816    0.003657
    8          1             0       -2.711825    0.775630    0.005863
```



10 triplet

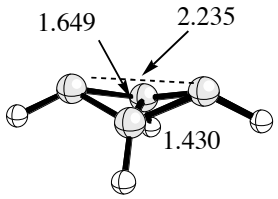
```
SCF Done:  E(UB+HF-LYP) =  -154.721909586     A.U. after    1 cycles
             Convg  =    0.1869D-08             -V/T =  2.0050
             S**2   =   2.0512


Dipole moment (field-independent basis, Debye):
    X=    -1.3511    Y=     0.3329    Z=     0.0001  Tot=     1.3915

1                    2                    3
                     A                    A                    A
 Frequencies --   -17.5681              104.8127             128.7487

Zero-point correction=                           0.055300 (Hartree/Particle)
 Thermal correction to Enthalpy=                 0.061704
Sum of electronic and zero-point Energies=          -154.666609 (42.6)
 Sum of electronic and thermal Energies=            -154.661150
 Sum of electronic and thermal Enthalpies=          -154.660206 (43.2)
 Sum of electronic and thermal Free Energies=       -154.694695

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.127             16.211            72.588


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.878847    0.001500    0.000249
    2          1             0       -2.280677    1.014841   -0.089764
    3          1             0       -2.276616   -0.428662    0.924141
    4          1             0       -2.276556   -0.584544   -0.833510
    5          6             0       -0.432960    0.007151   -0.000720
    6          6             0        0.828377    0.012460    0.000228
    7          6             0        2.102359   -0.062505    0.000063
    8          1             0        3.120266    0.246737    0.000213
 ---------------------------------------------------------------------
 Rotational constants (GHZ):    155.8898667      3.8085107      3.8055324
```



11 collapses to 10

12

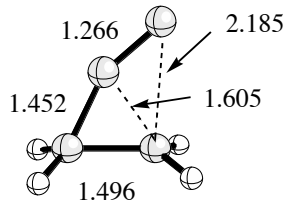
```
SCF Done:  E(RB+HF-LYP) =  -154.705668657     A.U. after    8 cycles
             Convg  =    0.5535D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                      A                     A                     A
 Frequencies --   520.4254              604.0400              689.9292

Zero-point correction=                           0.060203 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.645466 (55.8)
 Sum of electronic and thermal Energies=            -154.641770
 Sum of electronic and thermal Enthalpies=          -154.640826 (55.3)
 Sum of electronic and thermal Free Energies=       -154.670609

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.097             12.750            62.684

Dipole moment (field-independent basis, Debye):
    X=     0.0002    Y=     0.0001    Z=     2.6794  Tot=     2.6794

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.117409    0.000008   -0.260384
    2          6             0       -1.117410   -0.000036   -0.260401
    3          6             0       -0.000044    0.824389    0.083192
    4          6             0        0.000041   -0.824394    0.083195
    5          1             0       -2.078969   -0.000064    0.230378
    6          1             0       -0.000039    1.610105    0.832785
    7          1             0        0.000033   -1.609899    0.832906
    8          1             0        2.079000    0.000050    0.230321
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     20.4204874     12.0640194      8.3930218
```



13

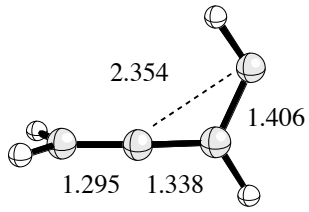
```
SCF Done:  E(RB+HF-LYP) =  -154.705261739     A.U. after    8 cycles
             Convg  =    0.8418D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A'                    A"                    A'
 Frequencies --   141.6610              261.0660              740.4298

Zero-point correction=                           0.061291 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.643970
```

```
 Sum of electronic and thermal Energies=             -154.639588
 Sum of electronic and thermal Enthalpies=           -154.638644
 Sum of electronic and thermal Free Energies=        -154.670140

                    E (Thermal)             CV                S
                     Kcal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  41.211             13.589            66.291

Dipole moment (field-independent basis, Debye):
    X=    -3.1865    Y=    -3.0199    Z=     0.0000  Tot=     4.3902

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.249706   -0.908616    0.000000
    2          6             0       -1.102216   -0.268850    0.000000
    3          6             0        0.000000    0.677036    0.000000
    4          6             0        1.207851    1.055174    0.000000
    5          1             0        0.618215   -1.330296    0.921654
    6          1             0        0.618215   -1.330296   -0.921654
    7          1             0       -1.684236   -0.333937   -0.911422
    8          1             0       -1.684236   -0.333937    0.911422
 ---------------------------------------------------------------------
```



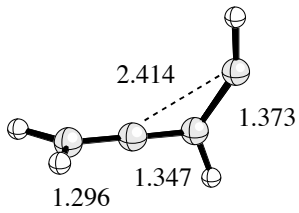
14a

```
SCF Done:  E(UB+HF-LYP) =  -154.694306064     A.U. after    1 cycles
             Convg  =    0.2686D-08             -V/T =  2.0050
             S**2   =   0.4558

1                    2                    3
                    ?A                   ?A                   ?A
 Frequencies --   163.4645             275.3881             408.2244

Zero-point correction=                           0.057174 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.637132 (61.0)
 Sum of electronic and thermal Energies=              -154.632333
 Sum of electronic and thermal Enthalpies=            -154.631388 (61.3)
 Sum of electronic and thermal Free Energies=         -154.663616

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  38.889             15.802            67.829

Dipole moment (Debye):
    X=    -2.8052    Y=     0.2520    Z=    -0.5029  Tot=     2.8610

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.720615   -0.183755    0.025545
    2          6             0       -0.493306    0.222605   -0.048892
    3          6             0        0.803572    0.549467   -0.014278
    4          6             0        1.748042   -0.490805    0.048132
    5          1             0        1.391855   -1.449367   -0.344060
    6          1             0        1.092947    1.580804    0.167884
    7          1             0       -2.387854   -0.108194   -0.825723
    8          1             0       -2.123109   -0.608320    0.938851
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     35.3490568      5.1551918      4.6464634
```



14a triplet

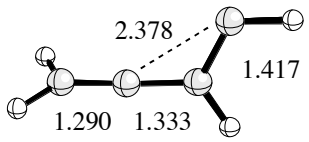
```
SCF Done:  E(UB+HF-LYP) =  -154.698255378     A.U. after    1 cycles
             Convg  =    0.3213D-08             -V/T =  2.0049
             S**2   =   2.0332


Dipole moment (field-independent basis, Debye):
    X=    -0.7376    Y=    -0.1650    Z=     0.0032  Tot=     0.7558

1                    2                    3
                     A                    A                    A
 Frequencies --   206.6815             211.6138             472.4888

Zero-point correction=                           0.057144 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.062906
 Sum of electronic and zero-point Energies=          -154.641111 (58.6)
 Sum of electronic and thermal Energies=             -154.636294
 Sum of electronic and thermal Enthalpies=           -154.635350 (58.8)
 Sum of electronic and thermal Free Energies=        -154.668589

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   38.881            15.935            69.959


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.780868   -0.185382    0.000777
    2          6             0       -0.529300    0.152584   -0.002566
    3          6             0        0.771990    0.502310    0.000527
    4          6             0        1.825763   -0.377595    0.000325
    5          1             0        1.944368   -1.448994   -0.000895
    6          1             0        0.999187    1.567634    0.001909
    7          1             0       -2.337098   -0.334864   -0.920978
    8          1             0       -2.331965   -0.335278    0.925588
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     42.2523638      4.7660515      4.4114203
```



14b

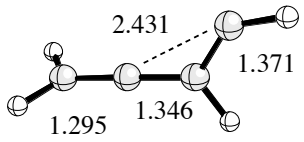
```
SCF Done:  E(UB+HF-LYP) =  -154.691969592     A.U. after   20 cycles
             Convg  =    0.4652D-08             -V/T =  2.0050
             S**2   =   0.4837

1                    2                    3
                    ?A                   ?A                   ?A
 Frequencies --   158.1799             210.5088             410.2746
```

```
Zero-point correction=                           0.056439 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.635531 (62.1)
Sum of electronic and thermal Enthalpies=            -154.629598 (62.4)
Sum of electronic and thermal Free Energies=         -154.662162

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  38.546             16.267            68.537

Dipole moment (Debye):
    X=    -1.7659    Y=     1.7640    Z=     0.3769  Tot=     2.5243

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.790034   -0.167871    0.013660
    2          6             0       -0.539719    0.149519   -0.016337
    3          6             0        0.755088    0.465445   -0.006488
    4          6             0        1.728357   -0.563471   -0.040949
    5          1             0        2.737955   -0.206791    0.196677
    6          1             0        1.005464    1.527126    0.055956
    7          1             0       -2.368050   -0.245177   -0.900247
    8          1             0       -2.297520   -0.376891    0.948302
 ---------------------------------------------------------------------
```



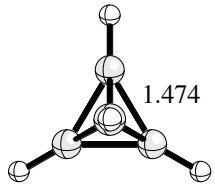
14b triplet

```
SCF Done:  E(UB+HF-LYP) =  -154.698149281     A.U. after    1 cycles
             Convg  =    0.8044D-09             -V/T =  2.0049
             S**2   =   2.0349

Dipole moment (field-independent basis, Debye):
    X=    -0.0513    Y=     0.7356    Z=     0.0011  Tot=     0.7373


1                    2                    3
                     A                    A                    A
 Frequencies --   206.4157             216.5140             477.7868

Zero-point correction=                           0.056777 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.062586
Sum of electronic and zero-point Energies=           -154.641372 (58.4)
 Sum of electronic and thermal Energies=             -154.636508
 Sum of electronic and thermal Enthalpies=           -154.635564 (58.6)
 Sum of electronic and thermal Free Energies=        -154.668786

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.681             16.163            69.923

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.829609   -0.159275    0.000348
    2          6             0       -0.563652    0.114729   -0.001111
    3          6             0        0.747701    0.417722    0.000245
    4          6             0        1.797496   -0.464633    0.000135
    5          1             0        2.870558   -0.367979    0.000176
    6          1             0        0.996538    1.483588    0.000126
    7          1             0       -2.390255   -0.284142   -0.922336
    8          1             0       -2.388462   -0.282730    0.924336
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     54.0723218      4.5119818      4.2858642
```



15

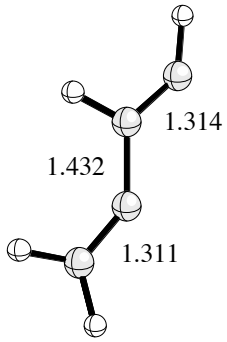
```
SCF Done:  E(RB+HF-LYP) =  -154.694445452     A.U. after    9 cycles
             Convg  =    0.2868D-08             -V/T =  2.0051
             S**2   =   0.0000

1                      2                      3
                      A'                     A"                     A'
 Frequencies --   571.4476               571.6613               776.3987

Zero-point correction=                           0.059474 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.634971 (62.4)
 Sum of electronic and thermal Energies=             -154.631160
 Sum of electronic and thermal Enthalpies=           -154.630216 (61.9)
 Sum of electronic and thermal Free Energies=        -154.660021

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   39.712             13.736            62.731

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.300978    0.851269    0.000000
    2          6             0        0.902948    0.000027    0.000000
    3          6             0       -0.300978   -0.425647    0.737214
    4          6             0       -0.300978   -0.425647   -0.737214
    5          1             0       -0.656952    1.858205    0.000000
    6          1             0        1.970950    0.000153    0.000000
    7          1             0       -0.657043   -0.929185    1.609176
    8          1             0       -0.657043   -0.929185   -1.609176
 ---------------------------------------------------------------------
```



16

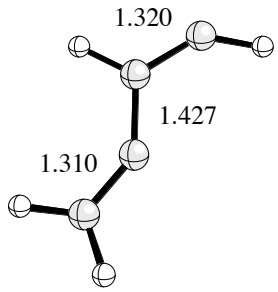
```
SCF Done:  E(UB+HF-LYP) =  -154.680180105     A.U. after   11 cycles
             Convg  =    0.6511E-08             -V/T =  2.0049
             S**2   =   0.9850

1                      2                      3
                      A"                     A'                     A"
 Frequencies --   106.3340               228.5245               428.4734

Zero-point correction=                           0.056449 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.623731 (69.5)
 Sum of electronic and thermal Energies=             -154.618664
 Sum of electronic and thermal Enthalpies=           -154.617720 (69.8)
 Sum of electronic and thermal Free Energies=        -154.650414

                        E                  CV                S
                   KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
```

```
 TOTAL                  38.602             16.320             68.811

Dipole moment (Debye):
    X=     1.1271    Y=    -0.7604    Z=     0.0000  Tot=     1.3596

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          6           0.972603    1.559384    0.000000
    2          6           0.000000    0.680122    0.000000
    3          6          -0.134597   -0.745754    0.000000
    4          6          -1.209375   -1.500993    0.000000
    5          1          -1.402842   -2.561322    0.000000
    6          1           0.827821   -1.277292    0.000000
    7          1           0.782694    2.626067    0.000000
    8          1           2.020540    1.255993    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     75.9178642      4.3941615      4.1537410
```



17

```
SCF Done:  E(UB+HF-LYP) =  -154.678986187     A.U. after   10 cycles
             Convg  =    0.8389E-08             -V/T =  2.0049
             S**2   =   0.9974

1                      2                      3
                      A'                     A"                     A'
 Frequencies --   111.8664               124.2177               420.3125


Zero-point correction=                           0.056553 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.622433 (70.3)
 Sum of electronic and thermal Energies=              -154.617225
 Sum of electronic and thermal Enthalpies=            -154.616281 (70.7)
 Sum of electronic and thermal Free Energies=         -154.649558

                        E                CV                S
                    KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  38.756             16.260             70.037

Dipole moment (Debye):
    X=    -0.3280    Y=     0.2412    Z=     0.0000  Tot=     0.4072

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          6          -0.772438    1.633169    0.000000
    2          6           0.000000    0.575370    0.000000
    3          6          -0.059515   -0.850313    0.000000
    4          6           1.029855   -1.595547    0.000000
    5          1           2.095888   -1.430362    0.000000
    6          1          -1.043438   -1.326605    0.000000
    7          1          -0.379786    2.643177    0.000000
    8          1          -1.860079    1.537712    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     55.2766551      4.6646021      4.3016048
```



18 collapses to 14b

19 collapses to 3

20

SCF Done: E(RB+HF-LYP) = -154.681562888   A.U. after   9 cycles
             Convg =   0.4866D-08   -V/T = 2.0050
             S**2   =   0.0000

1	2	3
	A	A	A
Frequencies --	366.1530	401.9689	713.0159

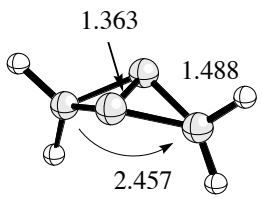
Zero-point correction=   0.061905 (Hartree/Particle)
Sum of electronic and zero-point Energies=   -154.619658 (72.0)
 Sum of electronic and thermal Energies=   -154.615824
 Sum of electronic and thermal Enthalpies=   -154.614880 (71.6)
 Sum of electronic and thermal Free Energies=   -154.644937

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	41.252	12.425	63.260

Dipole moment (field-independent basis, Debye):
    X=   -0.0002   Y=   -0.0327   Z=   0.8399 Tot=   0.8405

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000177	-0.673422	-0.321401
2	6	0	1.228586	-0.004942	0.185952
3	6	0	0.000174	0.689176	-0.292712
4	6	0	-1.228631	-0.004991	0.185962
5	1	0	2.053604	0.009423	-0.510658
6	1	0	1.523359	-0.027369	1.237086
7	1	0	-2.053831	0.010009	-0.510374
8	1	0	-1.522845	-0.026991	1.237139

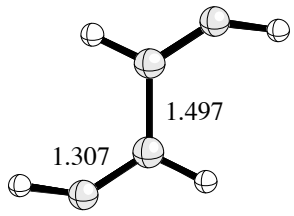


21

SCF Done: E(UB+HF-LYP) = -154.677406490   A.U. after   10 cycles
             Convg =   0.6232E-08   -V/T = 2.0049
             S**2   =   0.9569

1	2	3

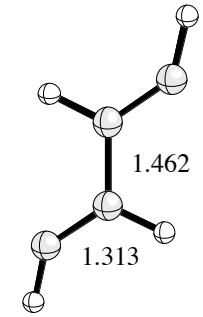
```
                     AU                     BU                     AG
 Frequencies --   144.0731               315.3994               438.3164

Zero-point correction=                           0.057318 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.620088 (71.7)
 Sum of electronic and thermal Energies=              -154.615352
 Sum of electronic and thermal Enthalpies=            -154.614408 (71.9)
 Sum of electronic and thermal Free Energies=         -154.645807

                        E                     CV                    S
                    KCAL/MOL          CAL/MOL-KELVIN      CAL/MOL-KELVIN
 TOTAL                 38.939              15.748              66.084

Dipole moment (Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          6           0.329599    1.800966    0.000000
    2          6          -0.329599    0.671962    0.000000
    3          6           0.329599   -0.671962    0.000000
    4          6          -0.329599   -1.800966    0.000000
    5          1          -1.350506   -2.145419    0.000000
    6          1           1.414229   -0.664925    0.000000
    7          1          -1.414229    0.664925    0.000000
    8          1           1.350506    2.145419    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     45.8005672      5.0168191      4.5215462
```



22

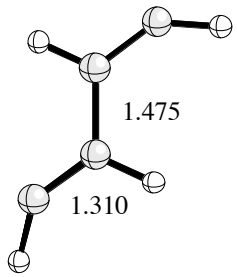
```
SCF Done:  E(UB+HF-LYP) =  -154.676259417     A.U. after   10 cycles
             Convg  =    0.5293E-08             -V/T =  2.0049
             S**2   =   1.0374

1                    2                    3
                     AU                     BU                     AG
 Frequencies --   180.3734               304.9686               509.1570

Zero-point correction=                           0.057083 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.619177 (72.3)
 Sum of electronic and thermal Energies=              -154.614500
 Sum of electronic and thermal Enthalpies=            -154.613556 (72.4)
 Sum of electronic and thermal Free Energies=         -154.644660

                        E                     CV                    S
                    KCAL/MOL          CAL/MOL-KELVIN      CAL/MOL-KELVIN
 TOTAL                 38.755              15.750              65.463

Dipole moment (Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000

---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------

    1          6           0.597707    1.733464    0.000000
    2          6           0.597707    0.420586    0.000000
    3          6          -0.597707   -0.420586    0.000000
    4          6          -0.597707   -1.733464    0.000000
    5          1          -1.319547   -2.532623    0.000000
    6          1          -1.554081    0.107118    0.000000
    7          1           1.554081   -0.107118    0.000000
```

```
    8          1           1.319547    2.532623    0.000000
 ---------------------------------------------------------------
```



23

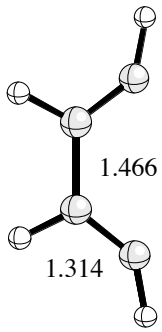
```
SCF Done:  E(UB+HF-LYP) =  -154.675563498     A.U. after    9 cycles
             Convg  =    0.6804E-08             -V/T =  2.0049
             S**2   =   1.0254
1                      2                      3
                      A"                    A'                     A'
 Frequencies --   163.8682               306.9415               476.2831

Zero-point correction=                           0.057117 (Hartree/Particle)
 Sum of electronic and zero-point Energies=          -154.618446 (72.8)
 Sum of electronic and thermal Energies=             -154.613730
 Sum of electronic and thermal Enthalpies=           -154.612786 (72.9)
 Sum of electronic and thermal Free Energies=        -154.644700

                        E                 CV                 S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  38.801             15.802             67.169

Dipole moment (Debye):
    X=     0.6748    Y=     0.9611    Z=     0.0000  Tot=     1.1743

Standard orientation:
 ---------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------
    1          6           0.984860   -1.568542    0.000000
    2          6          -0.060534   -0.776722    0.000000
    3          6           0.000000    0.697500    0.000000
    4          6          -1.046165    1.485296    0.000000
    5          1          -1.269987    2.538048    0.000000
    6          1           0.999611    1.136020    0.000000
    7          1          -1.058620   -1.205405    0.000000
    8          1           2.060032   -1.493855    0.000000
 ---------------------------------------------------------------
 Rotational constants (GHZ):     52.3501305      4.8708957      4.4562645
```



24

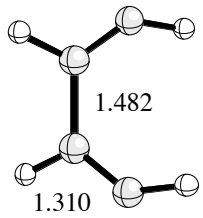
```
SCF Done:  E(UB+HF-LYP) =  -154.671368716     A.U. after    1 cycles
             Convg  =    0.1499E-08             -V/T =  2.0049
             S**2   =   1.0348

1                      2                      3
                      A                      A                      B
 Frequencies --   108.3922               262.9959               428.0780
```

```
 Zero-point correction=                           0.056693
 Sum of electronic and zero-point Energies=           -154.614676 (75.1)
 Sum of electronic and thermal Energies=              -154.609809
 Sum of electronic and thermal Enthalpies=            -154.608865 (75.4)
 Sum of electronic and thermal Free Energies=         -154.640763

                        E                 CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  38.629             15.935            67.135

Dipole moment (Debye):
    X=     0.0000    Y=     0.0000    Z=     1.1190  Tot=     1.1190
?ero
-------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
-------------------------------------------------------------
    1          6           0.000000    1.514052   -0.583926
    2          6           0.000000    0.733241    0.472336
    3          6           0.000000   -0.733241    0.472336
    4          6           0.000000   -1.514052   -0.583926
    5          1           0.000000   -2.571598   -0.788547
    6          1           0.000000   -1.205684    1.458085
    7          1           0.000000    1.205684    1.458085
    8          1           0.000000    2.571598   -0.788547
-------------------------------------------------------------
```



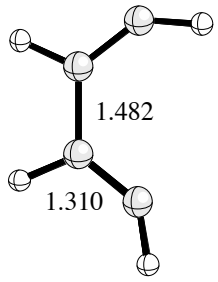
25

```
SCF Done:  E(UB+HF-LYP) =  -154.672310259     a.u. after    3 cycles
            Convg  =    0.2188D-06                  22 Fock formations.
              S**2 =  0.9361                  -V/T =  2.0049

1                     2                     3
                      A                     A                     B
 Frequencies --   108.2292              263.4400              427.9846

Zero-point correction=                           0.056688 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.615622 (74.5)
 Sum of electronic and thermal Energies=             -154.610723
 Sum of electronic and thermal Enthalpies=           -154.609778 (74.8)
 Sum of electronic and thermal Free Energies=        -154.641794

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.647             16.072            67.382

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=     0.1268  Tot=     0.1268

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.420930    1.536727    0.462342
    2          6             0       -0.420930    0.631842   -0.470086
    3          6             0        0.420930   -0.631842   -0.470086
    4          6             0        0.420930   -1.536727    0.462342
    5          1             0       -0.042260   -1.725174    1.415908
    6          1             0        1.019885   -0.757322   -1.369449
    7          1             0       -1.019885    0.757322   -1.369449
    8          1             0        0.042260    1.725174    1.415908
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     23.8954847      6.0151198      5.0854214
```



26

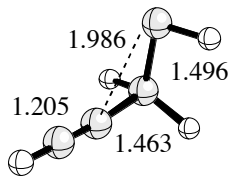
```
SCF Done:  E(UB+HF-LYP) =  -154.670838370     A.U. after   11 cycles
             Convg  =    0.7598E-08             -V/T =  2.0049
             S**2   =   1.0383

1                     2                     3
                     A"                    A'                    A'
 Frequencies --   -77.4125              261.7138              527.6767

Zero-point correction=                           0.056623 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.614215 (75.4)
 Sum of electronic and thermal Energies=             -154.610086
 Sum of electronic and thermal Enthalpies=           -154.609142 (75.2)
 Sum of electronic and thermal Free Energies=        -154.640152

                          E                     CV                S
                      KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                   38.122             13.939             65.266

Dipole moment (Debye):
    X=     0.1735    Y=     0.9845    Z=     0.0000  Tot=     0.9997

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          6          -0.459945   -1.608988    0.000000
    2          6          -0.854410   -0.359242    0.000000
    3          6           0.000000    0.851874    0.000000
    4          6           1.307802    0.924573    0.000000
    5          1           2.064334    1.690422    0.000000
    6          1          -0.557631    1.792331    0.000000
    7          1          -1.922534   -0.154932    0.000000
    8          1           0.455152   -2.177125    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     24.6616121      6.1371831      4.9142451
```



27a

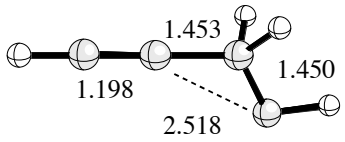
```
SCF Done:  E(RB+HF-LYP) =  -154.662898488     A.U. after    9 cycles
             Convg  =    0.3875D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A                     A                     A
 Frequencies --   145.3953              303.5734              377.4849

Zero-point correction=                           0.058102 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.604797 (81.3)
 Sum of electronic and thermal Energies=             -154.600027
 Sum of electronic and thermal Enthalpies=           -154.599082 (81.5)
```

```
 Sum of electronic and thermal Free Energies=         -154.631285

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.453             15.612             67.776

Dipole moment (field-independent basis, Debye):
    X=    -1.0862    Y=    -1.5489    Z=     1.5296  Tot=     2.4328

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.627870    0.084327   -0.000287
    2          1             0       -2.636687    0.416521   -0.019024
    3          6             0       -0.499466   -0.337111    0.004577
    4          6             0        0.943995   -0.576255    0.022735
    5          1             0        1.256838   -1.178848   -0.828876
    6          6             0        1.040540    0.902058   -0.184195
    7          1             0        0.976320    1.349401    0.821943
    8          1             0        1.260330   -1.025187    0.968984
 ---------------------------------------------------------------------
```



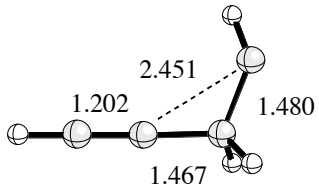
27b

```
SCF Done:  E(RB+HF-LYP) =  -154.662844808     A.U. after    9 cycles
             Convg  =    0.3026D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                      A                     A                     A
 Frequencies --   196.5358              253.6345              335.8594


Zero-point correction=                           0.056170 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.606675 (80.2)
 Sum of electronic and thermal Energies=            -154.601746
 Sum of electronic and thermal Enthalpies=          -154.600802 (80.4)
 Sum of electronic and thermal Free Energies=       -154.633136

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.340             16.390             68.053

Dipole moment (field-independent basis, Debye):
    X=     0.0801    Y=     2.4285    Z=    -0.0494  Tot=     2.4303

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.902557   -0.167991   -0.011633
    2          1             0        2.935729   -0.410897   -0.023303
    3          6             0        0.731650    0.086528   -0.000306
    4          6             0       -0.678689    0.435062   -0.014390
    5          1             0       -1.031660    0.611023    1.053842
    6          6             0       -1.688940   -0.605323   -0.023954
    7          1             0       -0.860093    1.388089   -0.526110
    8          1             0       -2.643442   -0.077875   -0.202731
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     46.3047587      4.6515036      4.3318855
```



27b triplet

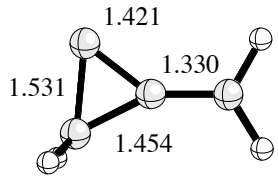
```
SCF Done:  E(UB+HF-LYP) =  -154.658143340     A.U. after    1 cycles
             Convg  =    0.1390D-08             -V/T =  2.0045
             S**2   =   2.0060

Dipole moment (field-independent basis, Debye):
    X=     0.1452    Y=    -0.3177    Z=     0.4768  Tot=     0.5911

1                    2                    3
                     A                    A                    A
 Frequencies --   148.8730             236.4827             323.3795

Zero-point correction=                          0.057265 (Hartree/Particle)
 Thermal correction to Enthalpy=                0.063275
Sum of electronic and zero-point Energies=          -154.600879 (83.6)
 Sum of electronic and thermal Energies=            -154.595813
 Sum of electronic and thermal Enthalpies=          -154.594869 (84.2)
 Sum of electronic and thermal Free Energies=       -154.628728

                    E (Thermal)             CV               S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.113            16.540            71.263


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.822190    0.229770   -0.009268
    2          1             0        2.832564    0.558330   -0.023218
    3          6             0        0.681007   -0.148928    0.003079
    4          6             0       -0.721540   -0.577841    0.027408
    5          1             0       -0.895496   -1.299260   -0.781912
    6          6             0       -1.664405    0.554674   -0.107954
    7          1             0       -0.910493   -1.132016    0.961701
    8          1             0       -1.730085    1.526895    0.363842
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     31.4749030      5.0810576      4.5157626
```



28

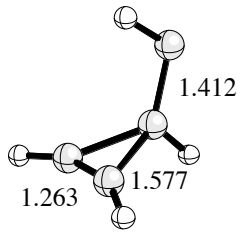
```
SCF Done:  E(UB+HF-LYP) =  -154.682428795     A.U. after   12 cycles
             Convg  =    0.9561D-08             -V/T =  2.0050
             S**2   =   0.1482

1                    2                    3
                     A                    A                    A
 Frequencies --   130.0239             333.4532             333.9858

Zero-point correction=                          0.057754 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.624674 (68.9)
 Sum of electronic and thermal Energies=            -154.619936
 Sum of electronic and thermal Enthalpies=          -154.618992 (69.0)
 Sum of electronic and thermal Free Energies=       -154.651116

                    E (Thermal)             CV               S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
```

```
 Total                   39.215             15.251             67.610

Dipole moment (field-independent basis, Debye):
    X=     1.6089    Y=    -2.4099    Z=     0.0002  Tot=     2.8976

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.223057    0.019007   -0.000090
    2          6             0        1.546582   -0.116434    0.000004
    3          6             0       -1.127643   -0.519528    0.000018
    4          6             0       -0.822459    0.981224    0.000034
    5          1             0       -1.565408   -0.933299    0.906994
    6          1             0        2.035160   -1.083642   -0.000056
    7          1             0        2.178798    0.764399    0.000150
    8          1             0       -1.565770   -0.933070   -0.906887
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     25.3406900      7.3969668      5.9491394
```



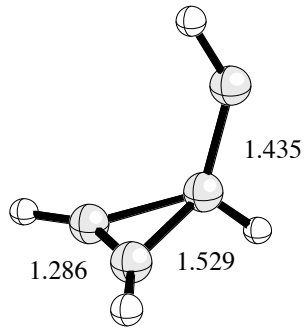
29

```
SCF Done:  E(UB+HF-LYP) =  -154.649940566     A.U. after   13 cycles
             Convg  =    0.5922D-08             -V/T =  2.0050
             S**2   =   0.2794

1                     2                     3
                      A                     A                     A
 Frequencies --    190.1250              461.5650              537.5999

Zero-point correction=                           0.056984 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.592957 (88.8)
Sum of electronic and thermal Enthalpies=            -154.587500 (88.8)
 Sum of electronic and thermal Free Energies=         -154.618971

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.590             15.605             66.237

Dipole moment (field-independent basis, Debye):
    X=    -3.7387    Y=     0.0001    Z=    -0.4354  Tot=     3.7640

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.383926   -0.000418    0.501902
    2          6             0        1.599414    0.000066   -0.216329
    3          6             0       -0.920567   -0.631340   -0.119938
    4          6             0       -0.920298    0.631629   -0.119452
    5          1             0       -1.334831   -1.606273   -0.283530
    6          1             0       -1.333918    1.606892   -0.282693
    7          1             0        1.399089    0.000374   -1.298100
    8          1             0        0.414808   -0.000615    1.587223
 ---------------------------------------------------------------------
```



29 triplet

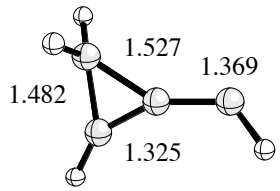
```
SCF Done:  E(UB+HF-LYP) =  -154.645143851     A.U. after    1 cycles
             Convg  =    0.2006D-08             -V/T =  2.0049
             S**2   =   2.0092

Dipole moment (field-independent basis, Debye):
    X=    -1.3704    Y=     0.0003    Z=    -0.4859  Tot=     1.4540

1                     2                     3
                      A                     A                     A
 Frequencies --   242.5987              359.7588              424.8538


Zero-point correction=                           0.056977 (Hartree/Particle)
 Thermal correction to Enthalpy=                 0.062481
Sum of electronic and zero-point Energies=          -154.588167 (91.8)
 Sum of electronic and thermal Energies=            -154.583607
 Sum of electronic and thermal Enthalpies=          -154.582662 (91.8)
 Sum of electronic and thermal Free Energies=       -154.615200

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.615             15.690            68.482


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.323701   -0.000106    0.514576
    2          6             0        1.572393   -0.000027   -0.192353
    3          6             0       -0.910088   -0.643116   -0.120443
    4          6             0       -0.909941    0.643213   -0.120305
    5          1             0       -1.347067   -1.577797   -0.424235
    6          1             0       -1.346772    1.578082   -0.423736
    7          1             0        1.838491    0.000255   -1.239719
    8          1             0        0.398957   -0.000324    1.598844
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     21.6029205      7.6027160      6.9255918
```



30

```
SCF Done:  E(UB+HF-LYP) =  -154.655794316     A.U. after    1 cycles
             Convg  =    0.1112D-08             -V/T =  2.0050
             S**2   =   0.8550

Dipole moment (field-independent basis, Debye):
```

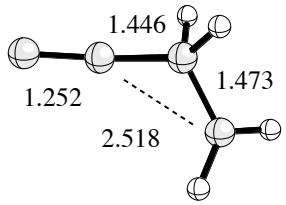
```
    X=    -1.6210    Y=    -1.4011    Z=     0.0000  Tot=     2.1426

1                      2                      3
                      A"                     A'                     A'
 Frequencies --    332.0728               333.1429               639.7553

Zero-point correction=                           0.059349 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.064450
Sum of electronic and zero-point Energies=           -154.596446 (86.6)
 Sum of electronic and thermal Energies=             -154.592289
 Sum of electronic and thermal Enthalpies=           -154.591344 (86.4)
 Sum of electronic and thermal Free Energies=        -154.622223

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.850             13.993            64.990

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.834077   -0.692947    0.000000
    2          6             0        0.000000    0.336342    0.000000
    3          6             0        0.599993   -1.068342    0.000000
    4          1             0       -1.850954   -1.047957    0.000000
    5          6             0        0.276118    1.676944    0.000000
    6          1             0       -0.502528    2.436984    0.000000
    7          1             0        1.050637   -1.450506    0.913252
    8          1             0        1.050637   -1.450506   -0.913252
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     23.9892593      7.4693023      5.9201805
```



32

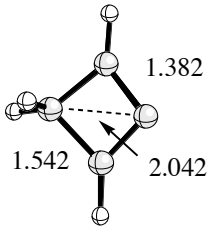
```
SCF Done:  E(UB+HF-LYP) =  -154.635203306     A.U. after   25 cycles
             Convg  =    0.3143D-08             -V/T =  2.0049
             S**2   =   0.8342

1                      2                      3
                      A                      A                      A
 Frequencies --    163.6329               188.6734               268.9163

Zero-point correction=                           0.055730 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.579473 (97.2)
 Sum of electronic and thermal Energies=             -154.574215
 Sum of electronic and thermal Enthalpies=           -154.573271 (97.7
 Sum of electronic and thermal Free Energies=        -154.606455

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.271             16.709            69.841

Dipole moment (field-independent basis, Debye):
    X=     4.4548    Y=     1.2130    Z=     0.5923  Tot=     4.6548

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.056147   -0.305023   -0.106064
    2          6             0       -0.877934    0.049268    0.123603
    3          6             0        0.478654    0.537226    0.014473
    4          6             0        1.589291   -0.428938   -0.027845
    5          1             0        1.456960   -1.449067    0.298444
    6          1             0        0.633161    1.205510    0.885252
    7          1             0        0.547430    1.240631   -0.827395
```

```
   8          1             0        2.559262   -0.112277   -0.381297
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     36.1429912      4.8584953      4.4355782
```



33

```
SCF Done:  E(UB+HF-LYP) =  -154.686113959     A.U. after    1 cycles
             Convg  =    0.2444D-08             -V/T =  2.0049
             S**2   =   1.0427


                      1                      2                      3
                      A                      A                      A
 Frequencies --   414.3719               469.5316               543.0716

Zero-point correction=                           0.059583 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.626531 (67.7)
 Sum of electronic and thermal Energies=            -154.622606
 Sum of electronic and thermal Enthalpies=          -154.621662 (67.4)
 Sum of electronic and thermal Free Energies=       -154.651921

E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.852             13.423             63.685

Dipole moment (field-independent basis, Debye):
    X=    -0.0015    Y=     1.3729    Z=    -0.0011  Tot=     1.3729


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.002065    0.963097    0.000115
    2          6             0        1.043604   -0.170512    0.000205
    3          6             0        0.001737   -1.078778    0.000251
    4          6             0       -1.042636   -0.173123   -0.000389
    5          1             0        2.118826   -0.201158   -0.001652
    6          1             0       -0.002509    1.582924   -0.898341
    7          1             0       -0.002384    1.582745    0.898739
    8          1             0       -2.117769   -0.208612    0.000156
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     15.5872262     13.7381727      7.6625588
```



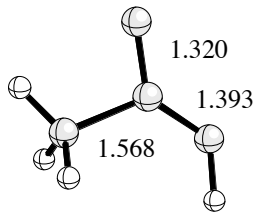
35 collapses to 20

36 collapses to 13a

37 collapses to 3

38

```
SCF DONE:  E(UB+HF-LYP) =  -154.608186455     A.U. AFTER   15 CYCLES
             CONVG  =    0.6801D-08             -V/T =  2.0048
             S**2   =   0.6724

1                    2                    3
                     A                    A                    A
 Frequencies --   141.3777             221.4646             310.8579
Zero-point correction=                           0.055615 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.552571 (114.1)
 Sum of electronic and thermal Energies=            -154.547256
 Sum of electronic and thermal Enthalpies=          -154.546312 (114.6)
 Sum of electronic and thermal Free Energies=       -154.579611

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.234             16.996             70.084

Dipole moment (field-independent basis, Debye):
    X=    -1.5104    Y=    -2.7392    Z=     0.4222  Tot=     3.1564

Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.259960    1.421564    0.042890
    2          6             0        0.232255    0.198863   -0.031661
    3          6             0        1.524725   -0.320966   -0.064925
    4          6             0       -1.083451   -0.653865   -0.005489
    5          1             0       -1.982104   -0.034044   -0.018609
    6          1             0        1.678497   -1.308986    0.374448
    7          1             0       -1.087179   -1.257498    0.898539
    8          1             0       -1.090628   -1.273050   -0.899266
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     13.4522737      9.2901444      5.7239340
```



39 collapses to 6

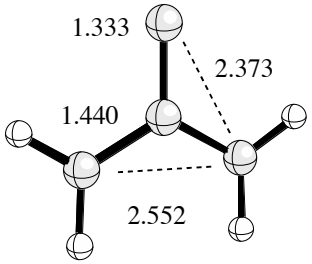
40

```
SCF Done:  E(UB+HF-LYP) =  -154.630347855     A.U. after    1 cycles
             Convg  =    0.8138D-10             -V/T =  2.0048
             S**2   =   0.9819

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=    -2.1374  Tot=     2.1374

                   1                    2                    3
                   B1                   B2                   A2
 Frequencies --  -600.8484             154.3638             191.9354

 Zero-point correction=                           0.053357 (Hartree/Particle)
 Thermal correction to Enthalpy=                  0.059539

 Sum of electronic and zero-point Energies=          -154.576991 (98.8)
 Sum of electronic and thermal Enthalpies=           -154.570809 (99.3)

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  36.769             16.850             68.398
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.466191
2	6	0	0.000000	0.000000	0.133207
3	6	0	0.000000	1.276183	-0.534548
4	6	0	0.000000	-1.276183	-0.534548
5	1	0	0.000000	-2.198609	0.022404
6	1	0	0.000000	1.307869	-1.613315
7	1	0	0.000000	-1.307869	-1.613315
8	1	0	0.000000	2.198609	0.022404

Rotational constants (GHZ): 13.3264179 9.6670226 5.6027624



41

Rotation gradient small -- convergence achieved.
SCF Done: E(UB+HF-LYP) = -154.590241251 a.u. after 3 cycles
Convg = 0.1725D-06 25 Fock formations.
S**2 = 0.5593 -V/T = 2.0048

1	2	3
A	A	A
Frequencies -- 118.7448	146.2867	305.0947

Zero-point correction= 0.053536 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.536705 (124.1)
Sum of electronic and thermal Energies= -154.531247
Sum of electronic and thermal Enthalpies= -154.530302 (124.7)
Sum of electronic and thermal Free Energies= -154.564091

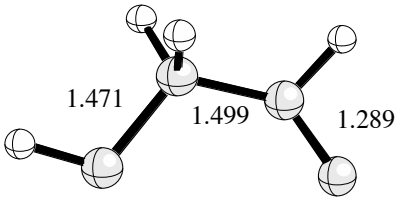
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	37.020	17.318	71.114

Dipole moment (field-independent basis, Debye):
X= -2.3523 Y= 3.7094 Z= 0.0000 Tot= 4.3924

Standard orientation:

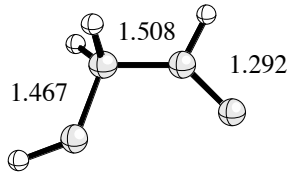
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.849116	0.313014	0.000000
2	6	0	1.719446	-0.637163	0.000000
3	6	0	-0.635349	0.521392	0.000000
4	1	0	1.534538	1.183463	0.000000
5	6	0	-1.458150	-0.697684	0.000000
6	1	0	-0.927906	1.138883	-0.865250
7	1	0	-0.927906	1.138883	0.865250
8	1	0	-2.529102	-0.458582	0.000000

Rotational constants (GHZ): 24.3910619 5.8488801 4.8543773



41 triplet

```
SCF Done:  E(UB+HF-LYP) =  -154.592103742     A.U. after    1 cycles
             Convg  =    0.1488D-08             -V/T =  2.0048
             S**2   =   2.0063

1                      2                      3
                      A"                     A'                     A"
 Frequencies --    118.8303               120.4447               138.0598

Zero-point correction=                           0.054465 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.061072
Sum of electronic and zero-point Energies=           -154.537638 (123.5)
 Sum of electronic and thermal Energies=             -154.531976
 Sum of electronic and thermal Enthalpies=           -154.531032 (124.2)
 Sum of electronic and thermal Free Energies=        -154.566595

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  37.731             17.112            74.848


Dipole moment (field-independent basis, Debye):
    X=    -0.6637    Y=     3.5814    Z=     0.0000  Tot=     3.6423

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.831821   -0.407731    0.000000
    2          6             0       -0.581670   -1.674788    0.000000
    3          6             0        0.000000    0.849750    0.000000
    4          1             0       -1.929412   -0.329839    0.000000
    5          6             0        1.445348    0.598044    0.000000
    6          1             0       -0.286511    1.447901    0.877248
    7          1             0       -0.286511    1.447901   -0.877248
    8          1             0        2.311290    1.242382    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     22.0278037      6.2301172      5.0057779
```



42 collapses to 4

43 collapses to 39

Decomposition products

H2

```
SCF Done:  E(RB+HF-LYP) =  -1.18003403252     A.U. after    4 cycles
             Convg  =    0.1654D-08             -V/T =  2.0362
             S**2   =   0.0000

1
                    SGG
 Frequencies --  4410.4885

Zero-point correction=                           0.010048 (Hartree/Particle)
Sum of electronic and zero-point Energies=             -1.169986
 Sum of electronic and thermal Energies=               -1.167626
 Sum of electronic and thermal Enthalpies=             -1.166682
 Sum of electronic and thermal Free Energies=          -1.181473

                       E                CV                S
                   KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 7.786             4.968             31.132

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          1           0.000000    0.000000    0.371368
    2          1           0.000000    0.000000   -0.371368
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.0000000   1817.9999185   1817.9999185
```

H

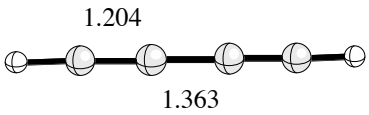
```
SCF Done:  E(UB+HF-LYP) = -0.502256981542     A.U. after    6 cycles
             Convg  =    0.1580D-10             -V/T =  2.0117
             S**2   =   0.7500

Sum of electronic and zero-point Energies=             -0.502257
 Sum of electronic and thermal Energies=               -0.500841
 Sum of electronic and thermal Enthalpies=             -0.499897
 Sum of electronic and thermal Free Energies=          -0.512911

                       E                CV                S
                   KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 0.889             2.981             27.392
```

DP1

```
SCF Done:  E(RB+HF-LYP) =  -153.542624329     A.U. after    8 cycles
             Convg  =    0.2893D-08             -V/T =  2.0049
             S**2   =   0.0000

1                    2                    3
                   PIU                  PIU                  PIG
 Frequencies --   240.3199             240.3199             571.6205

Zero-point correction=                           0.037807 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -153.504817 (37.4)
 Sum of electronic and thermal Energies=             -153.500573
 Sum of electronic and thermal Enthalpies=           -153.499629 (39.3)
 Sum of electronic and thermal Free Energies=        -153.527522

E                CV                S
                   KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                26.387            14.652             58.705

Dipole moment (Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000

Largest concise Abelian subgroup C2      NOp   2
                  Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          1           0.000000    0.000000    2.947078
```

2	6	0.000000	0.000000	1.885753
3	6	0.000000	0.000000	0.681592
4	6	0.000000	0.000000	-0.681592
5	6	0.000000	0.000000	-1.885753
6	1	0.000000	0.000000	-2.947078

Rotational constants (GHZ): 0.0000000 4.4330882 4.4330882



DP2 (Acetylene)

SCF Done: E(RB+HF-LYP) = -77.3623375005 A.U. after 6 cycles
Convg = 0.4393D-09 -V/T = 2.0051
S**2 = 0.0000

1	2	3
	PIG	PIG	PIU
Frequencies --	653.4711	653.4711	761.3051

Zero-point correction= 0.026936 (Hartree/Particle)
Sum of electronic and zero-point Energies= -77.335402 (39.9)
Sum of electronic and thermal Energies= -77.332595
Sum of electronic and thermal Enthalpies= -77.331651 (41.2)
Sum of electronic and thermal Free Energies= -77.354353

	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	18.664	8.252	47.781

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	0.598140
2	6	0.000000	0.000000	-0.598140
3	1	0.000000	0.000000	-1.659867
4	1	0.000000	0.000000	1.659867

Rotational constants (GHZ): 0.0000000 35.7412583 35.7412583

DP2a

SCF Done: E(RB+HF-LYP) = -154.725944052 A.U. after 12 cycles
Convg = 0.8202E-08 -V/T = 2.0051
S**2 = 0.0000

1	2	3
	B2	A1	B1
Frequencies --	30.6221	55.2935	58.8818

Zero-point correction= 0.054496 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.671448 (39.5)
Sum of electronic and thermal Energies= -154.664492
Sum of electronic and thermal Enthalpies= -154.663547 (41.1)
Sum of electronic and thermal Free Energies= -154.702818

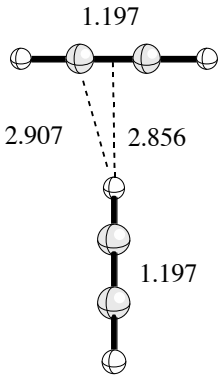
	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	38.562	20.272	82.651

Dipole moment (Debye):
X= 0.0000 Y= 0.0000 Z= -0.3226 Tot= 0.3226

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.598276	-2.253110

2	1	0.000000	0.000000	0.591619
3	6	0.000000	-0.598276	-2.253110
4	1	0.000000	1.660373	-2.257939
5	1	0.000000	-1.660373	-2.257939
6	6	0.000000	0.000000	1.655555
7	6	0.000000	0.000000	2.852368
8	1	0.000000	0.000000	3.914035



DP3

SCF Done: E(RB+HF-LYP) = -153.476486525 A.U. after 33 cycles
Convg = 0.9649E-08 -V/T = 2.0048
S**2 = 0.0000

1	2	3
B2	B1	B2
Frequencies -- 162.2004	207.7708	430.5041

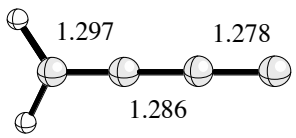
Zero-point correction= 0.035654 (Hartree/Particle)
Sum of electronic and zero-point Energies= -153.440832 (77.6)
Sum of electronic and thermal Energies= -153.436165
Sum of electronic and thermal Enthalpies= -153.435221 (79.7)
Sum of electronic and thermal Free Energies= -153.465773

	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	25.302	13.960	64.302

Dipole moment (Debye):
X= 0.0000 Y= 0.0000 Z= -4.6189 Tot= 4.6189

Standard orientation:

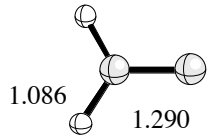
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	2.117392
2	6	0.000000	0.000000	0.839496
3	6	0.000000	0.000000	-0.446873
4	6	0.000000	0.000000	-1.743886
5	1	0.000000	0.930206	-2.298387
6	1	0.000000	-0.930206	-2.298387



DP4 (Vinylidene)

SCF Done: E(RB+HF-LYP) = -77.2933651387 A.U. after 11 cycles
Convg = 0.4783D-08 -V/T = 2.0048
S**2 = 0.0000

```
1                      2                      3
                      B2                     B1                     A1
 Frequencies --    344.0345               756.8778              1215.4017

Zero-point correction=                           0.023584 (Hartree/Particle)
Sum of electronic and zero-point Energies=            -77.269781 (81.1)
Exp. Value                                             82.6
 Sum of electronic and thermal Energies=              -77.266471
 Sum of electronic and thermal Enthalpies=            -77.265527 (82.7)
 Sum of electronic and thermal Free Energies=         -77.290778

                        E                     CV                    S
                    KCAL/MOL          CAL/MOL-KELVIN      CAL/MOL-KELVIN
 TOTAL                 16.876                 8.504              53.145

Dipole moment (Debye):
    X=     0.0000    Y=     0.0000    Z=    -2.5139  Tot=     2.5139

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number              X           Y           Z
 ---------------------------------------------------------------------
    1          6           0.000000    0.000000    0.815569
    2          6           0.000000    0.000000   -0.474431
    3          1           0.000000    0.937025   -1.023412
    4          1           0.000000   -0.937025   -1.023412
 ---------------------------------------------------------------------
 Rotational constants (GHZ):    285.5613414     39.9969014     35.0830276
```

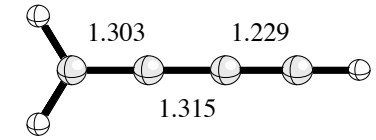


DP5 collapses to DP1

DP6

```
SCF Done:  E(UB+HF-LYP) =  -154.130168304     a.u. after   28 cycles
           Convg  =    0.5302E-07                   163 Fock formations.
 Annihilation of the first spin contaminant:
 S**2 before annihilation     0.7772,   after     0.7505

1                      2                      3
                      A'                     A"                     A'
 Frequencies --    104.9117               230.2502               319.8839

Zero-point correction=                           0.045346 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.084823 (92.4)
 Sum of electronic and thermal Energies=             -154.079563
 Sum of electronic and thermal Enthalpies=           -154.078618 (94.4)
 Sum of electronic and thermal Free Energies=        -154.111686

                        E                     CV                    S
                    KCAL/MOL          CAL/MOL-KELVIN      CAL/MOL-KELVIN
 TOTAL                 31.756                16.420              69.598

Dipole moment (Debye):
    X=    -0.0005    Y=     0.0981    Z=     0.0000  Tot=     0.0981

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number              X           Y           Z
 ---------------------------------------------------------------------
    1          6           0.000123    1.864949    0.000000
    2          6           0.000000    0.562420    0.000000
    3          6          -0.000068   -0.752271    0.000000
    4          6          -0.000017   -1.981287    0.000000
    5          1          -0.000581   -3.042206    0.000000
    6          1           0.923248    2.439576    0.000000
    7          1          -0.922889    2.439757    0.000000
```

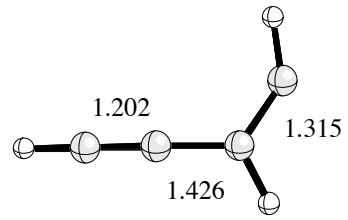
```
 ---------------------------------------------------------
 Rotational constants (GHZ):     294.2620904      4.1874644      4.1287112
```



DP7 rearranges to DP6

DP8a

```
SCF Done:  E(UB+HF-LYP) =  -154.104680774     a.u. after    3 cycles
            Convg  =    0.1741D-06                   29 Fock formations.
              S**2 =  0.7631                  -V/T =  2.0049

1                     2                     3
                      A                     A                     A
 Frequencies --    214.1111              343.0663              511.6746

Zero-point correction=                           0.047210 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.057470 (109.4)
 Sum of electronic and thermal Energies=             -154.052969
 Sum of electronic and thermal Enthalpies=           -154.052025 (111.1)
 Sum of electronic and thermal Free Energies=        -154.084088

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  32.450             14.925             67.482

Dipole moment (field-independent basis, Debye):
    X=     0.2311    Y=    -0.2920    Z=     0.0014  Tot=     0.3723

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.723592   -0.369130    0.000053
    2          6             0       -0.731650    0.493681   -0.000019
    3          6             0        0.642965    0.115898   -0.000062
    4          6             0        1.806747   -0.184802   -0.000182
    5          1             0        2.832740   -0.455908    0.001015
    6          1             0       -0.943571    1.560678    0.000277
    7          1             0       -1.855998   -1.438656   -0.000031
 ---------------------------------------------------------------------
Rotational constants (GHZ):     51.1586144      5.1223219      4.6561219
```



DP8b

```
SCF Done:  E(UB+HF-LYP) =  -154.104647433     a.u. after    3 cycles
            Convg  =    0.1772D-06                   28 Fock formations.
              S**2 =  0.7632                  -V/T =  2.0049

1                     2                     3
                      A                     A                     A
 Frequencies --    224.1279              332.7344              532.2770
```

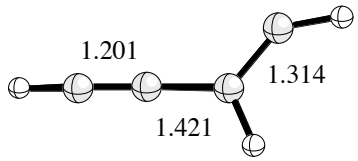
Zero-point correction= 0.046926 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.057722 (109.3)
Sum of electronic and thermal Energies= -154.053208
Sum of electronic and thermal Enthalpies= -154.052264 (111.0)
Sum of electronic and thermal Free Energies= -154.084227

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	32.279	15.050	67.271

Dipole moment (field-independent basis, Debye):
X= -0.5233 Y= 0.6412 Z= 0.0003 Tot= 0.8276

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.697415	-0.447391	0.000002
2	6	0	-0.702791	0.411255	-0.000004
3	6	0	0.679261	0.079100	-0.000013
4	6	0	1.856723	-0.159321	-0.000038
5	1	0	2.894664	-0.379983	0.000222
6	1	0	-0.935582	1.480055	0.000058
7	1	0	-2.773748	-0.401933	0.000041

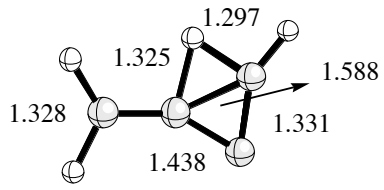


DP9 (2 x vinylidene)

Transition States

TS(1,2)

```
SCF Done:  E(RB+HF-LYP) =  -154.645528591     A.U. after    7 cycles
Convg  =    0.9913D-08             -V/T =  2.0050
S**2   =   0.0000

1                     2                     3
A                     A                     A
Frequencies --  -779.8100               147.0814               405.2539


Sum of electronic and zero-point Energies=           -154.591112 (89.9)
Sum of electronic and thermal Energies=              -154.586623
Sum of electronic and thermal Enthalpies=            -154.585679 (89.9)
Sum of electronic and thermal Free Energies=         -154.617236

                       E (Thermal)             CV               S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                    36.964             14.576             66.418


Dipole moment (field-independent basis, Debye):
X=    -0.7190    Y=     3.5786    Z=     0.0059  Tot=     3.6501

Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
1          6             0        1.249669    0.424152   -0.002123
2          1             0        2.005412    1.185479    0.123335
3          6             0        0.927336   -0.866929    0.009564
4          6             0       -0.263147   -0.059797   -0.000908
5          1             0        0.197851    1.180372   -0.073708
6          6             0       -1.583177    0.071914    0.001777
7          1             0       -2.096266    1.018363    0.037882
8          1             0       -2.162952   -0.839495   -0.037615
---------------------------------------------------------------------
```



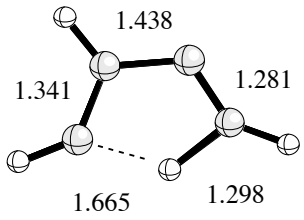
TS(1,3)

```
SCF Done:  E(UB+HF-LYP) =  -154.636251567 (99.9)     a.u. after   10 cycles
            Convg  =    0.1066D-06                   87 Fock formations.
              S**2 =  0.6575                  -V/T =  2.0049

1                     2                     3
                      A                     A                     A
 Frequencies -- -2098.0879               441.3634               469.2992

Zero-point vibrational energy     138629.0 (Joules/Mol)
                                   33.13314 (Kcal/Mol)
Sum of electronic and zero-point Energies=           -154.583451
 Sum of electronic and thermal Energies=              -154.579361
 Sum of electronic and thermal Enthalpies=            -154.578416 (94.5)
 Sum of electronic and thermal Free Energies=         -154.609135

                      E (Thermal)             CV               S
                       KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                    35.700             14.247             64.653

Dipole moment (field-independent basis, Debye):
    X=    -0.5055    Y=    -0.2486    Z=     0.0000  Tot=     0.5633
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.205966	-0.663683	0.000003
2	6	0	-0.739364	0.593688	-0.000006
3	6	0	0.694262	0.699158	-0.000005
4	6	0	1.394377	-0.373340	0.000004
5	1	0	2.399782	-0.748219	0.000014
6	1	0	0.377242	-1.179847	0.000017
7	1	0	-1.417536	1.441300	-0.000010
8	1	0	-2.219342	-1.048171	0.000001

Rotational constants (GHZ): 22.8744996 7.6417607 5.7281414



TS(1,4)

SCF Done: E(UB+HF-LYP) = -154.636583865 A.U. after 18 cycles
Convg = 0.4157D-08 -V/T = 2.0050
S**2 = 0.0000

1	2	3
	A	A	A
Frequencies --	-1282.9619	299.9448	408.3525

Zero-point correction= 0.055503 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.581081
Sum of electronic and thermal Energies= -154.576975
Sum of electronic and thermal Enthalpies= -154.576031 (96.0)
Sum of electronic and thermal Free Energies= -154.606746

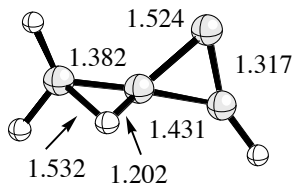
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	37.405	13.649	64.645

Dipole moment (field-independent basis, Debye):
X= -2.3308 Y= -3.1717 Z= 0.3866 Tot= 3.9550

Standard orientation:

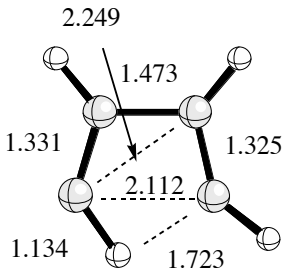
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.229988	-0.419826	-0.092431
2	1	0	1.862132	-1.285343	-0.183229
3	6	0	0.973867	0.862842	0.059298
4	6	0	-0.168115	-0.146000	0.040148
5	1	0	-0.694344	-0.692705	0.972568
6	6	0	-1.533813	0.007022	-0.101728
7	1	0	-1.977013	0.999181	-0.135022
8	1	0	-2.202337	-0.845364	-0.086045

Rotational constants (GHZ): 30.9251019 7.0109281 5.8845397



TS(1,5)

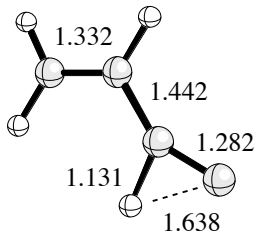
```
SCF Done:  E(RB+HF-LYP) =  -154.637717780     A.U. after    1 cycles
             Convg  =    0.5617D-09             -V/T =  2.0049
             S**2   =   0.0000

Dipole moment (field-independent basis, Debye):
    X=     1.6186    Y=     0.8263    Z=     0.0000  Tot=     1.8173

                     1                      2                      3
                     A                      A                      A
 Frequencies -- -1011.5770               245.8600               466.2798

 Zero-point correction=                           0.055593 (Hartree/Particle)
 Thermal correction to Enthalpy=                  0.060784

 Sum of electronic and zero-point Energies=           -154.582125 (95.6)
 Sum of electronic and thermal Enthalpies=            -154.576934 (95.4)

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 37.550             14.198             65.200

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.849894    0.520102   -0.000013
    2          6             0        0.606984    0.738843    0.000028
    3          6             0        1.065808   -0.504600    0.000024
    4          6             0       -1.036016   -0.797423   -0.000043
    5          1             0       -1.651893    1.244904   -0.000026
    6          1             0        1.176865    1.666218    0.000048
    7          1             0        2.005272   -1.037007    0.000023
    8          1             0       -0.251535   -1.615651   -0.000020
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     17.7958628     10.5311365      6.6159729
```



TS(1,6)

```
SCF Done:  E(RB+HF-LYP) =  -154.719659905     A.U. after    8 cycles
             Convg  =    0.4857D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                      3
                    A'                     A"                     A'
 Frequencies --  -157.5249               193.9737               393.5682

Zero-point correction=                           0.057438 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.662222 (45.3)
```

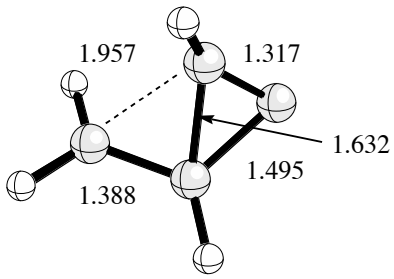
```
 Sum of electronic and thermal Energies=             -154.657885
 Sum of electronic and thermal Enthalpies=           -154.656941 (45.2)
 Sum of electronic and thermal Free Energies=        -154.688210

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.764             13.924            65.812

Dipole moment (field-independent basis, Debye):
    X=     2.1630    Y=     2.1354    Z=     0.0000  Tot=     3.0395

Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.270694    1.108338    0.000000
    2          6             0        0.000000    0.709975    0.000000
    3          6             0       -0.438791   -0.663610    0.000000
    4          6             0       -1.348777   -1.566002    0.000000
    5          1             0        2.092646    0.405234    0.000000
    6          1             0        1.520392    2.159158    0.000000
    7          1             0       -0.800381    1.439032    0.000000
    8          1             0        0.288585   -1.535628    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     55.4749023      4.7492482      4.3747247
```



TS (1,9)

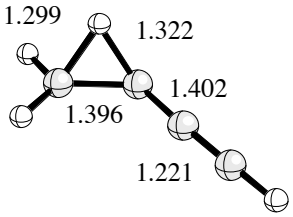
```
SCF Done:  E(RB+HF-LYP) =  -154.687033132     A.U. after    1 cycles
             Convg  =    0.2226D-08             -V/T =  2.0050
             S**2   =   0.0000

Dipole moment (field-independent basis, Debye):
    X=     3.1105    Y=     1.3461    Z=    -1.6034  Tot=     3.7494

1                    2                    3
                     A                    A                    A
 Frequencies --  -530.1863               469.3269              620.4025

Zero-point correction=                          0.059383 (Hartree/Particle)
Thermal correction to Enthalpy=                 0.063962
Sum of electronic and zero-point Energies=          -154.627650 (67.0)
 Sum of electronic and thermal Energies=            -154.624015
 Sum of electronic and thermal Enthalpies=          -154.623071 (66.5)
 Sum of electronic and thermal Free Energies=       -154.652921

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.544             12.056            62.824

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.205909    0.157149    0.162909
    2          6             0        0.159509   -0.699085   -0.150347
    3          6             0       -1.206261   -0.346394    0.343481
    4          6             0       -0.637101    0.725374   -0.167129
    5          1             0        1.253702    0.636496    1.125903
    6          1             0        2.088313    0.220050   -0.467208
    7          1             0        0.241745   -1.433369   -0.946891
    8          1             0       -0.716096    1.554562   -0.845284
```

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      20.8117991      9.7382883      7.7287235
```



TS(1,10)

```
SCF Done:  E(RB+HF-LYP) =  -154.681617861     A.U. after   11 cycles
             Convg  =    0.6090D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies -- -1189.1812               223.5323               281.2350

Zero-point correction=                           0.055182 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.626435 (67.8)
Sum of electronic and thermal Enthalpies=            -154.620930 (67.8)
Sum of electronic and thermal Free Energies=         -154.652534

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  37.490             14.834             66.516

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.916895    0.167097    0.014593
    2          1             0       -2.956526    0.406796    0.039173
    3          6             0       -0.731857   -0.124897   -0.012913
    4          6             0        0.586265   -0.590052   -0.119381
    5          1             0        1.326404   -0.448593    0.967209
    6          6             0        1.637757    0.324056   -0.029816
    7          1             0        2.663331   -0.030938   -0.138718
    8          1             0        1.515167    1.415509    0.017432
 ---------------------------------------------------------------------

Dipole moment (field-independent basis, Debye):
    X=     1.1137    Y=     1.7897    Z=     0.7662  Tot=     2.2429
```



TS(1,14b)

```
SCF Done:  E(RB+HF-LYP) =  -154.660621948     A.U. after   10 cycles
             Convg  =    0.8089D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -798.4711               227.0206               229.9590
```

Zero-point correction= 0.053512 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.607110 (79.9)
Sum of electronic and thermal Energies= -154.602368
Sum of electronic and thermal Enthalpies= -154.601423 (80.1)
Sum of electronic and thermal Free Energies= -154.633085

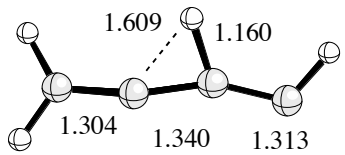
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	36.555	15.692	66.638

Dipole moment (field-independent basis, Debye):
X= -2.8380 Y= 2.1657 Z= -0.0215 Tot= 3.5700

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.018185	-0.233853	-0.044266
2	1	0	2.735788	0.577430	-0.139557
3	6	0	0.743701	0.064823	0.052555
4	6	0	-0.583741	-0.112260	0.017709
5	1	0	0.386213	1.142115	0.292956
6	6	0	-1.882522	-0.009562	-0.032046
7	1	0	-2.402024	0.918985	-0.237859
8	1	0	-2.493712	-0.893411	0.120748

Rotational constants (GHZ): 116.8417231 4.1381162 4.0123895



TS(1,22)

SCF Done: E(UB+HF-LYP) = -154.639931280 a.u. after 1 cycles
Convg = 0.6795D-07 1 Fock formations.
S**2 = 0.5740

1	2	3
	A'	A"	A'
Frequencies --	-1805.7312	275.8735	354.8483

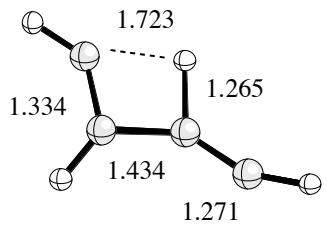
Zero-point correction= 0.052627 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.587304 (92.3)
Sum of electronic and thermal Enthalpies= -154.581959 (92.3)
Sum of electronic and thermal Free Energies= -154.613180

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	35.785	15.082	65.710

Standard orientation:

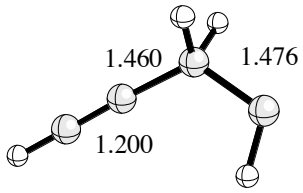
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.205720	1.824925	0.000000
2	1	0	-0.217784	2.807419	0.000000
3	6	0	0.000000	0.570819	0.000000
4	6	0	0.510299	-0.769048	0.000000
5	1	0	1.551003	-1.078678	0.000000
6	6	0	-0.600825	-1.507003	0.000000
7	1	0	-0.844569	-2.562573	0.000000
8	1	0	-1.179813	0.115671	0.000000

Dipole moment (field-independent basis, Debye):
X= 0.0881 Y= -0.2864 Z= 0.0000 Tot= 0.2996



TS(1,27a)

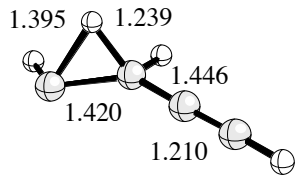
```
SCF Done:  E(RB+HF-LYP) =  -154.662949745     A.U. after   10 cycles
             Convg  =    0.4934D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -343.4438              212.6346              295.5093

Zero-point correction=                           0.056063 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.606887 (80.0)
Sum of electronic and thermal Enthalpies=           -154.601469 (80.0)
Sum of electronic and thermal Free Energies=        -154.633113

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   37.987             14.681             66.600

Dipole moment (field-independent basis, Debye):
    X=     1.6199    Y=    -0.5007    Z=     0.0019  Tot=     1.6955

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.825956   -0.199693    0.036911
    2          1             0        2.847923   -0.476601   -0.037600
    3          6             0        0.671466    0.115385    0.121444
    4          6             0       -0.747628    0.447605    0.210977
    5          1             0       -1.002685    1.311506   -0.425164
    6          6             0       -1.801897   -0.546289   -0.071659
    7          1             0       -1.006265    0.855378    1.202359
    8          1             0       -1.312847   -1.500507   -0.339820
 ---------------------------------------------------------------------
```



TS(1,27b)

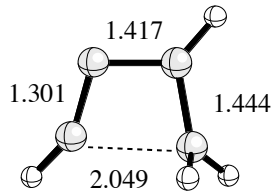
```
SCF Done:  E(RB+HF-LYP) =  -154.662599663     A.U. after    9 cycles
             Convg  =    0.4820D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
Frequencies --  -303.7328              227.6054              298.3425

Zero-point correction=                           0.055331 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.607269 (79.8)
Sum of electronic and thermal Enthalpies=           -154.601927 (79.4)
Sum of electronic and thermal Free Energies=        -154.633309

                     E (Thermal)             CV                S
```

```
                    KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 37.480             14.392             66.049

Dipole moment (field-independent basis, Debye):
    X=     0.6553    Y=     2.4961    Z=     0.2635  Tot=     2.5941

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.920631   -0.151740   -0.013881
    2          1             0        2.962678   -0.383845   -0.033891
    3          6             0        0.733866    0.081689    0.000927
    4          6             0       -0.671456    0.423001   -0.020717
    5          1             0       -0.846189    1.498420   -0.181864
    6          6             0       -1.704393   -0.549663   -0.081236
    7          1             0       -2.642356    0.031751   -0.150743
    8          1             0       -1.146027    0.033958    1.055939
 ---------------------------------------------------------------------
```



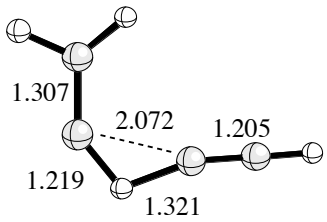
TS(1,33)

```
SCF Done:  E(UB+HF-LYP) =  -154.647573717     A.U. after    1 cycles
             Convg  =    0.4781D-08             -V/T =  2.0049
             S**2   =   0.7651

Dipole moment (field-independent basis, Debye):
    X=     0.8228    Y=    -1.4507    Z=    -0.5249  Tot=     1.7484


1                     2                     3
                      A                     A                     A
 Frequencies --  -871.2104              274.8373              404.5365

Zero-point correction=                           0.056104 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.591470
Sum of electronic and thermal Enthalpies=            -154.586262
Sum of electronic and thermal Free Energies=         -154.617243

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 37.881             14.351             65.204

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.861031   -0.736981    0.027273
    2          6             0        0.709924    0.697736   -0.026855
    3          6             0       -0.698008    0.799626    0.091401
    4          6             0       -1.161160   -0.409745   -0.030888
    5          1             0        1.437029    1.456102   -0.271046
    6          1             0        0.722916   -1.204796    0.993418
    7          1             0        1.489342   -1.294619   -0.667712
    8          1             0       -1.920013   -1.060500   -0.420247
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     16.7804972     10.6656336      6.8422626
```



TS(1,DP4)

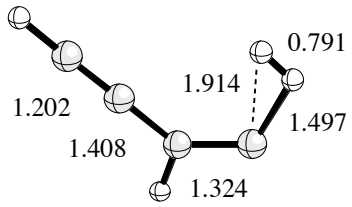
```
SCF Done:  E(RB+HF-LYP) =  -154.623293219     A.U. after    1 cycles
             Convg  =    0.4359D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A'                    A'                    A"
 Frequencies --  -1244.1897               132.9733              138.0910

Zero-point correction=                           0.052171 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.571123 (102.5)
 Sum of electronic and thermal Energies=            -154.565774
 Sum of electronic and thermal Enthalpies=          -154.564830 (103.0)
 Sum of electronic and thermal Free Energies=       -154.598556

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  36.094             17.020            70.983

Dipole moment (field-independent basis, Debye):
    X=     1.4254    Y=    -0.5580    Z=     0.0000  Tot=     1.5308

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.039864   -1.729188    0.000000
    2          6             0       -0.997227   -0.839156    0.000000
    3          6             0        0.000000    0.977202    0.000000
    4          6             0        0.858782    1.822506    0.000000
    5          1             0        1.613991    2.570914    0.000000
    6          1             0       -1.172159    0.367346    0.000000
    7          1             0       -0.398190   -2.755485    0.000000
    8          1             0        1.026209   -1.570959    0.000000
 ---------------------------------------------------------------------
```



TS(1,DP5) syn

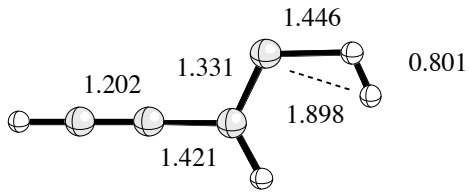
```
SCF Done:  E(RB+HF-LYP) =  -154.635780922     A.U. after    1 cycles
             Convg  =    0.2006D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A                     A                     A
 Frequencies --   -389.1278               208.2831              282.0750

Zero-point correction=                           0.049599 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.586182 (93.0)
 Sum of electronic and thermal Energies=            -154.581038
 Sum of electronic and thermal Enthalpies=          -154.580094 (93.4)
 Sum of electronic and thermal Free Energies=       -154.612691

                    E (Thermal)             CV                S
```

```
                    KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 34.352            17.968            68.607

Dipole moment (field-independent basis, Debye):
    X=    -1.7258    Y=     0.1883    Z=     0.0000  Tot=     1.7361

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.805377    0.133963    0.000000
    2          6             0        0.656503   -0.523711    0.000000
    3          6             0       -0.701693   -0.152696    0.000000
    4          6             0       -1.862643    0.158196   -0.000001
    5          1             0       -2.885669    0.440710    0.000004
    6          1             0        0.892395   -1.592938    0.000000
    7          1             0        1.685934    1.625809    0.000000
    8          1             0        0.922071    1.831907    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     39.6313349      4.8237540      4.3003358
```



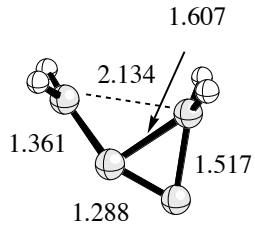
TS(1,DP5) anti

```
SCF Done:  E(RB+HF-LYP) =  -154.632253939     A.U. after    8 cycles
             Convg  =    0.6802D-08             -V/T =  2.0050
             S**2   =   0.0000

1    A   -389.1278   107.5557     1.0000

 Zero-point correction=                           0.049728
 Sum of electronic and zero-point Energies=           -154.582526  (95.3)
 Sum of electronic and thermal Energies=              -154.577336
 Sum of electronic and thermal Enthalpies=            -154.576392  (95.8)
 Sum of electronic and thermal Free Energies=         -154.608999

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 34.461            17.895            68.627

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.938222   -0.131626    0.000000
    2          6             0       -0.762831    0.117584    0.000000
    3          6             0        0.623993    0.428971    0.000000
    4          6             0        1.442713   -0.619988    0.000000
    5          1             0        0.910757    1.471602    0.000000
    6          1             0        2.860803   -0.338374    0.000000
    7          1             0        3.010985    0.448447    0.000000
    8          1             0       -2.976468   -0.351316    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     52.0487814      4.6505885      4.2691385
```



TS(2,13)

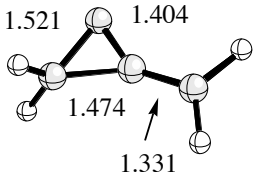
```
SCF Done:  E(RB+HF-LYP) =  -154.680295739     A.U. after   14 cycles
             Convg  =    0.4123D-08             -V/T =  2.0050
             S**2   =   0.0000
 KE= 1.539104749891D+02 PE=-5.533686203825D+02 EE= 1.470379249163D+02

1                      2                      3
                       A                      A                      A
 Frequencies --   -300.9161               302.2171               544.2811

Zero-point correction=                           0.059191 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.621105
 Sum of electronic and thermal Energies=             -154.617276
 Sum of electronic and thermal Enthalpies=           -154.616332 (70.7)
 Sum of electronic and thermal Free Energies=        -154.646595

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.546             12.429            63.694

Dipole moment (field-independent basis, Debye):
    X=     2.9300    Y=     2.5893    Z=     0.0000  Tot=     3.9102

Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.664229    0.773492    0.000000
    2          6             0        1.324531   -0.001200    0.000000
    3          6             0        0.117376   -0.630237    0.000000
    4          6             0       -1.170019   -0.656767    0.000000
    5          1             0       -0.672161    1.345573    0.923070
    6          1             0       -0.672161    1.345573   -0.923070
    7          1             0        1.849187    0.198559   -0.927103
    8          1             0        1.849187    0.198560    0.927103
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     20.9773201      9.3386952      7.0872240
```



TS(2,28)

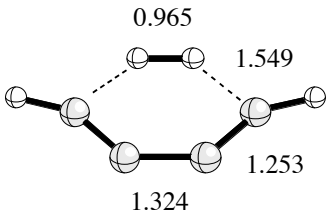
```
SCF Done:  E(UB+HF-LYP) =  -154.681835603     A.U. after    1 cycles
             Convg  =    0.4348D-08             -V/T =  2.0050
             S**2   =   0.0000


Zero-point correction=                           0.057651 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.062658
Sum of electronic and zero-point Energies=           -154.624185 (69.2)
```

```
 Sum of electronic and thermal Energies=             -154.620122
 Sum of electronic and thermal Enthalpies=           -154.619178 (68.9)
 Sum of electronic and thermal Free Energies=        -154.649934

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.726             13.235            64.731


Dipole moment (field-independent basis, Debye):
    X=     1.6803    Y=    -2.5288    Z=     0.3891  Tot=     3.0610


1                     2                     3
                      A                     A                     A
 Frequencies --  -262.8531              268.7910              390.7627


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.226591    0.062298   -0.066341
    2          6             0        1.544707   -0.114371   -0.006489
    3          6             0       -1.120424   -0.529266    0.024638
    4          6             0       -0.844810    0.966772    0.008146
    5          1             0       -1.756250   -0.876530   -0.786877
    6          1             0        2.009855   -1.075860   -0.185337
    7          1             0        2.191971    0.713567    0.259694
    8          1             0       -1.281956   -1.073778    0.952799
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     25.4075587      7.3953770      5.9576428
```



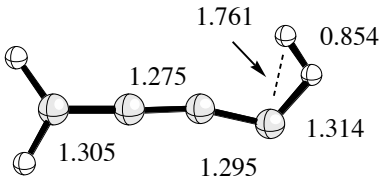
TS(2,DP1)

```
SCF Done:  E(RB+HF-LYP) =  -154.643982869     A.U. after   10 cycles
             Convg  =    0.6102D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A'                    A'                    A"
 Frequencies -- -1477.9812              409.9786              448.1350

Zero-point correction=                           0.050256 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.593727 (88.2)
Sum of electronic and thermal Enthalpies=           -154.588581  (88.1)
 Sum of electronic and thermal Free Energies=        -154.619430

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  34.173             14.814            64.927

Dipole moment (field-independent basis, Debye):
    X=     0.7052    Y=    -0.6662    Z=     0.0000  Tot=     0.9701

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.837466   -1.301933    0.000000
    2          6             0       -0.910011   -0.050609    0.000000
    3          6             0        0.000000    0.911208    0.000000
    4          6             0        1.253369    0.908745    0.000000
    5          1             0        1.374737   -0.636198    0.000000
    6          1             0        2.186260    1.431621    0.000000
    7          1             0       -1.307677   -2.262456    0.000000
    8          1             0        0.711325   -1.337431    0.000000
```



TS(2,DP3)

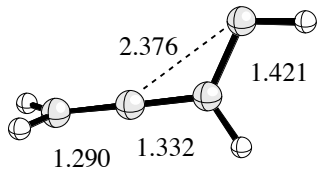
```
SCF Done:  E(RB+HF-LYP) =  -154.641243513     A.U. after    8 cycles
             Convg  =    0.7157D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -748.1440              203.5658              219.8814

Zero-point correction=                           0.049695 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.591548 (89.6)
Sum of electronic and thermal Enthalpies=           -154.585522 (90.0)
Sum of electronic and thermal Free Energies=        -154.617838

                      E (Thermal)             CV                S
                       KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                    34.373             17.004             68.013

Dipole moment (field-independent basis, Debye):
    X=     1.6540    Y=     1.3214    Z=     0.0000  Tot=     2.1170

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.943090    0.043150    0.000000
    2          6             0        0.638882    0.001787    0.000000
    3          6             0       -0.635940   -0.026206   -0.000001
    4          6             0       -1.890462   -0.347704    0.000000
    5          1             0       -2.857678    0.541827    0.000001
    6          1             0        2.533750   -0.865072    0.000001
    7          1             0        2.475629    0.986733    0.000001
    8          1             0       -2.485120    1.310351    0.000000
 ---------------------------------------------------------------------
```



TS(3,14b)

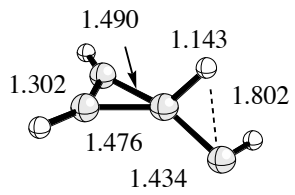
```
SCF Done:  E(UB+HF-LYP) =  -154.691939051     A.U. after   12 cycles
             Convg  =    0.4672D-08             -V/T =  2.0050
             S**2   =   0.4537

1                    2                    3
                    A"                   A'                   A"
 Frequencies --  -124.0812              217.2094              400.1699

Zero-point correction=                           0.056213 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.635726 (61.9)
Sum of electronic and thermal Enthalpies=           -154.630446 (61.8)
 Sum of electronic and thermal Free Energies=        -154.661744

                      E (Thermal)             CV                S
                       KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
```

```
 Total                   37.995             14.294             65.873

Dipole moment (field-independent basis, Debye):
    X=    -1.2667    Y=     2.2951    Z=     0.0000  Tot=     2.6215

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.641212    1.678571    0.000000
    2          6             0        0.000000    0.559377    0.000000
    3          6             0       -0.652512   -0.601342    0.000000
    4          6             0        0.087351   -1.814686    0.000000
    5          1             0       -0.562363   -2.699348    0.000000
    6          1             0       -1.744055   -0.555075    0.000000
    7          1             0        0.925055    2.161451    0.927830
    8          1             0        0.925055    2.161451   -0.927830
 ---------------------------------------------------------------------
```



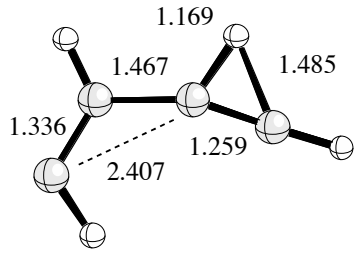
TS(3,29)

```
SCF Done:  E(UB+HF-LYP) =  -154.629431466     A.U. after    1 cycles
             Convg  =    0.4051D-09             -V/T =  2.0050
             S**2   =    0.2089

1                     2                     3
                      A                     A                     A
 Frequencies --  -699.7641              369.8777              503.9174

 Zero-point correction=                           0.054671 (Hartree/Particle)
 Sum of electronic and zero-point Energies=           -154.574760 (100.2)
 Sum of electronic and thermal Energies=              -154.570754
 Sum of electronic and thermal Enthalpies=            -154.569810 (99.9)
 Sum of electronic and thermal Free Energies=         -154.600361

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  36.820             13.835             64.299


 Dipole moment (field-independent basis, Debye):
    X=    -2.2810    Y=     1.4123    Z=     0.4683  Tot=     2.7234


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.666617   -0.159130   -0.238089
    2          6             0        0.319677   -0.022327    0.235743
    3          6             0       -0.993373   -0.631536   -0.053743
    4          6             0       -0.967598    0.670585   -0.050739
    5          1             0       -1.557626   -1.527931   -0.247438
    6          1             0       -1.488005    1.594861   -0.236933
    7          1             0        2.159844    0.826373   -0.175339
    8          1             0        0.733848   -0.038852    1.300679
 ---------------------------------------------------------------------
Rotational constants (GHZ):     26.2427995      7.1309326      6.0403677
```



TS(3,DP2)

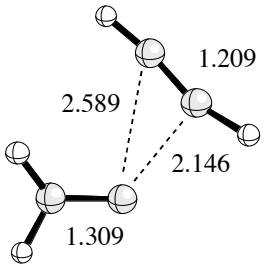
```
SCF Done:  E(RB+HF-LYP) =  -154.612682582     A.U. after    1 cycles
             Convg  =    0.6542D-08             -V/T =  2.0050
             S**2   =   0.0000

Dipole moment (field-independent basis, Debye):
    X=     5.9957    Y=     0.7554    Z=     0.2397  Tot=     6.0478

                    1                      2                      3
                    A                      A                      A
 Frequencies -- -1068.3358               42.3966               287.5896

 Zero-point correction=                           0.051618 (Hartree/Particle)
 Thermal correction to Enthalpy=                  0.057983

 Sum of electronic and zero-point Energies=           -154.561064 (108.8)
 Sum of electronic and thermal Enthalpies=            -154.554700 (109.4)

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  35.792             17.293             71.766

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.681126   -0.537987    0.004829
    2          6             0       -0.864424    0.518434   -0.019937
    3          6             0        0.583353    0.278342    0.010458
    4          6             0        1.692065   -0.315827   -0.029598
    5          1             0       -1.231973   -1.529063    0.088193
    6          1             0       -1.164254    1.555693   -0.072058
    7          1             0        1.375200    1.114609    0.210228
    8          1             0        2.641820   -0.799011   -0.020876
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     32.4286594      5.4234146      4.6526518
```



TS(3,DP4)

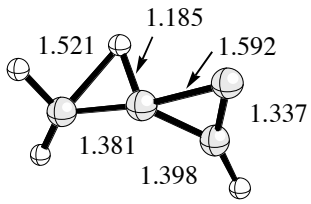
```
SCF Done:  E(RB+HF-LYP) =  -154.653080799     A.U. after   10 cycles
             Convg  =    0.7809D-08             -V/T =  2.0049
             S**2   =   0.0000
1                    2                      3
                     A                      A                      A
 Frequencies --  -248.3495               95.0543               189.8601

Zero-point correction=                           0.054126 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.598955 (85.0)
 Sum of electronic and thermal Energies=             -154.593598
 Sum of electronic and thermal Enthalpies=           -154.592653 (85.6)
```

```
 Sum of electronic and thermal Free Energies=         -154.626421

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 37.326             17.327             71.070

Dipole moment (field-independent basis, Debye):
    X=     0.4874    Y=     1.6850    Z=     0.9475  Tot=     1.9936

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.598157    0.306382    0.145945
    2          1             0       -2.656017    0.087525   -0.003553
    3          6             0       -0.839878   -0.640843   -0.345813
    4          6             0        1.237933   -0.532271    0.179350
    5          1             0       -1.348004    1.214990    0.669933
    6          6             0        1.401329    0.631642   -0.103068
    7          1             0        1.376221   -1.537696    0.493769
    8          1             0        1.420436    1.645726   -0.418634
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     21.2030883      5.2095131      4.4036435
```



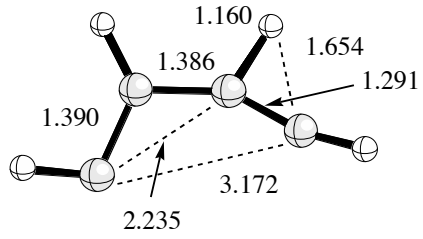
TS(4,6)

```
SCF Done:  E(RB+HF-LYP) =  -154.637909642     A.U. after    9 cycles
             Convg  =    0.5711D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies -- -1271.2978              278.1959              363.9076

Zero-point correction=                           0.055728 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.582182 (95.5)
 Sum of electronic and thermal Energies=            -154.578018
 Sum of electronic and thermal Enthalpies=          -154.577074 (95.3)
 Sum of electronic and thermal Free Energies=       -154.607935

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 37.583             13.711             64.952

Dipole moment (field-independent basis, Debye):
    X=    -3.1472    Y=     2.3470    Z=     0.7559  Tot=     3.9981

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.552789    0.060979   -0.081019
    2          6             0       -0.184052   -0.095800    0.012962
    3          6             0        1.040138    0.578198    0.047919
    4          1             0        1.456681    1.570115    0.013876
    5          6             0        1.272028   -0.729443   -0.105693
    6          1             0       -0.678112   -0.688009    0.912380
    7          1             0       -2.026818    1.038743   -0.067041
    8          1             0       -2.203701   -0.804452   -0.104230
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     31.1558187      6.8012969      5.7166480
```



TS(5,3)

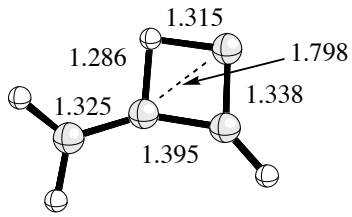
```
SCF Done:  E(RB+HF-LYP) =  -154.604592260     A.U. after    1 cycles
             Convg  =    0.8689D-09             -V/T =  2.0049
             S**2   =   0.0000

Dipole moment (field-independent basis, Debye):
    X=     4.0059    Y=     2.7564    Z=     1.0386  Tot=     4.9722

                     1                     2                     3
                     A                     A                     A
 Frequencies --  -652.5879              311.2276              360.6789

 Zero-point correction=                           0.053014 (Hartree/Particle)
 Thermal correction to Enthalpy=                  0.058457

 Sum of electronic and zero-point Energies=           -154.551579 (114.7)
 Sum of electronic and thermal Enthalpies=            -154.546136 (114.7)

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  36.090             15.313            66.309


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.503574   -0.676258   -0.000675
    2          6             0       -0.770421    0.504794   -0.002816
    3          6             0        0.604860    0.327074    0.016739
    4          6             0        1.654581   -0.410079   -0.123197
    5          1             0       -2.577118   -0.435747    0.073323
    6          1             0       -1.144767    1.529997    0.008035
    7          1             0        1.359679    1.206051    0.069111
    8          1             0        2.449533   -0.773482    0.509226
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     29.9994104      5.7513713      4.8658798
```



TS(6,3)

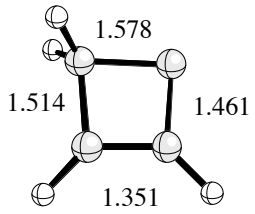
```
SCF Done:  E(RB+HF-LYP) =  -154.685314503     A.U. after   14 cycles
             Convg  =    0.7438D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                     3
                    ?A                    ?A                    ?A
 Frequencies --  -580.4070              363.8736              521.9287

Zero-point correction=                           0.056464 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.628851 (66.2)
 Sum of electronic and thermal Enthalpies=           -154.623990 (65.9)
 Sum of electronic and thermal Free Energies=        -154.654411
```

```
                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  37.889             13.219            64.025

Dipole moment (Debye):
    X=    -1.0713    Y=     1.4229    Z=     0.0000  Tot=     1.7811

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.611389   -0.002307    0.000008
    2          6             0       -0.286273   -0.019703   -0.000019
    3          6             0        0.959112    0.608048    0.000001
    4          6             0        1.395131   -0.656686    0.000008
    5          1             0        0.201966   -1.209815   -0.000014
    6          1             0        1.392181    1.589253    0.000011
    7          1             0       -2.204534   -0.903599    0.000015
    8          1             0       -2.129103    0.948047    0.000005
 ---------------------------------------------------------------------
```



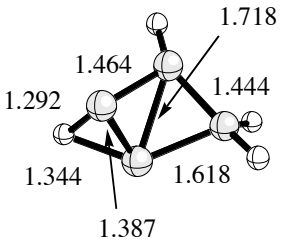
TS(7,7')

```
SCF Done:  E(RB+HF-LYP) =  -154.689317722     A.U. after    8 cycles
             Convg  =    0.6617D-08             -V/T =  2.0049
             S**2   =   0.0000

1                    2                    3
                    A"                   A"                   A'
 Frequencies --  -560.2018              671.9245              750.0041

Zero-point correction=                           0.060408 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.628910
 Sum of electronic and thermal Energies=             -154.625569
 Sum of electronic and thermal Enthalpies=           -154.624625 (65.5)
 Sum of electronic and thermal Free Energies=        -154.654052

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.003             10.629            61.935

Dipole moment (field-independent basis, Debye):
    X=     0.4958    Y=     3.4120    Z=     0.0000  Tot=     3.4478

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.038047   -0.167362    0.000000
    2          6             0       -0.212776   -1.129444    0.000000
    3          6             0       -1.041111    0.073859    0.000000
    4          1             0       -2.114278    0.206143    0.000000
    5          6             0        0.000000    0.935248    0.000000
    6          1             0        0.068371    2.025387    0.000000
    7          1             0        1.670473   -0.252669    0.884958
    8          1             0        1.670473   -0.252669   -0.884958
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     15.9110596     13.1496649      7.5386405
```



TS(7,9)

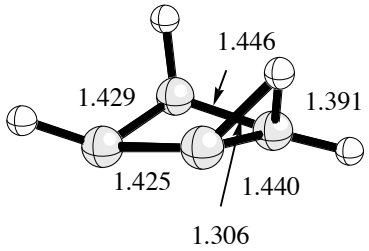
```
SCF Done:  E(RB+HF-LYP) =  -154.620048809     A.U. after    8 cycles
             Convg  =    0.9670D-08             -V/T =  2.0049
             S**2   =   0.0000


Dipole moment (field-independent basis, Debye):
    X=     2.7096    Y=     0.6077    Z=    -1.0390  Tot=     2.9649

1                    2                    3
                     A                    A                    A
 Frequencies -- -1510.0913               338.7025              547.6338

Zero-point correction=                           0.055816 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.564232
Sum of electronic and thermal Enthalpies=            -154.559483 (106.4)
Sum of electronic and thermal Free Energies=         -154.589532

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  37.413             12.520             63.244


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.172579    0.090277    0.335970
    2          6             0       -0.314771   -0.831447   -0.245651
    3          6             0        1.115842   -0.150699    0.083531
    4          6             0        0.054080    0.825591    0.020984
    5          1             0        0.076733    1.544228   -0.795105
    6          1             0        1.943479   -0.085566   -0.614870
    7          1             0        1.368778   -0.603274    1.033020
    8          1             0       -1.484420   -0.457717   -0.792045
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     20.5007614     11.1687764      8.3490948
```



TS(7,12)

```
SCF Done:  E(RB+HF-LYP) =  -154.621174029     A.U. after    1 cycles
             Convg  =    0.2295D-08             -V/T =  2.0049
             S**2   =   0.0000

Dipole moment (field-independent basis, Debye):
    X=     0.9660    Y=     1.1630    Z=     0.8336  Tot=     1.7265
1                    2                    3
                     A                    A                    A
```

```
 Frequencies --  -1552.0678               442.0264               617.2408

 Zero-point correction=                           0.055092 (Hartree/Particle)
 Thermal correction to Enthalpy=                  0.059756

 Sum of electronic and zero-point Energies=           -154.566082 (105.6)
 Sum of electronic and thermal Enthalpies=            -154.561418 (105.2)

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  36.905             12.545            62.825

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.075984    0.059519   -0.144557
    2          6             0        0.039991   -0.908301    0.111279
    3          6             0       -0.121814    0.858405   -0.001666
    4          6             0       -1.116517   -0.142989   -0.217454
    5          1             0       -2.119381   -0.168158    0.179311
    6          1             0       -0.212674    1.597927    0.795819
    7          1             0        0.970521   -0.716364    1.006304
    8          1             0        2.095667    0.086791   -0.467051
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     20.2488993     12.0840708      8.2641727
```

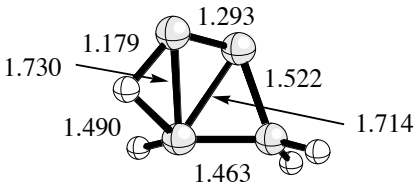


TS(7,13)

```
SCF Done:  E(RB+HF-LYP) =  -154.625389947     A.U. after    1 cycles
             Convg  =    0.3313D-08             -V/T =  2.0049
             S**2   =   0.0000


Dipole moment (field-independent basis, Debye):
    X=    -1.9957    Y=     1.2806    Z=     0.2378  Tot=     2.3831

                    1                      2                      3
                    A                      A                      A
 Frequencies --  -1308.6405              371.7696               528.0958

 Zero-point correction=                           0.056823 (Hartree/Particle)
 Thermal correction to Enthalpy=                  0.061595

 Sum of electronic and zero-point Energies=           -154.568567 (104.1)
 Sum of electronic and thermal Enthalpies=            -154.563795 (103.7)

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.059             12.693            63.336


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.207722   -0.785633   -0.329776
    2          6             0        1.276825   -0.221304    0.129554
    3          6             0       -1.093630   -0.151149    0.139043
    4          6             0       -0.056881    0.872815    0.009479
    5          1             0       -1.945023   -0.112242   -0.534692
```

6	1	0	-0.021971	1.472021	-0.894567
7	1	0	1.307058	0.855280	0.608292
8	1	0	-1.344281	-0.503434	1.131167

Rotational constants (GHZ): 20.3250963 10.9110434 8.0990837



TS(8,8')

SCF Done: E(UB+HF-LYP) = -154.644087505 A.U. after 1 cycles
Convg = 0.6836D-08 -V/T = 2.0049
S**2 = 0.0000

Dipole moment (field-independent basis, Debye):
X= 3.5746 Y= -1.2419 Z= 0.2593 Tot= 3.7931

1	2	3
A	A	A
Frequencies -- -602.0222	164.9081	218.8750

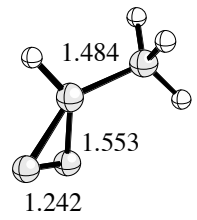
Zero-point correction= 0.057540 (Hartree/Particle)
Thermal correction to Enthalpy= 0.062991
Sum of electronic and zero-point Energies= -154.586548 (92.8)
Sum of electronic and thermal Energies= -154.582041
Sum of electronic and thermal Enthalpies= -154.581097 (92.8)
Sum of electronic and thermal Free Energies= -154.612853

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	38.935	13.657	66.837

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.050037	-0.430114	0.138654
2	6	0	1.427391	0.127369	-0.084412
3	6	0	-1.423602	-0.360859	-0.229188
4	6	0	-0.967570	0.790753	0.151366
5	1	0	1.424009	1.112721	-0.534063
6	1	0	0.134754	-1.449916	0.518043
7	1	0	1.971828	-0.581685	-0.716793
8	1	0	1.951870	0.155990	0.874293

Rotational constants (GHZ): 27.6723544 6.9895808 5.9779776

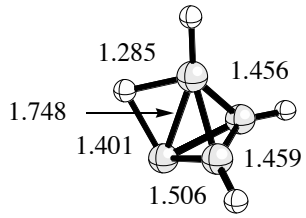


TS(9,15)

SCF Done: E(RB+HF-LYP) = -154.637725665 A.U. after 9 cycles
Convg = 0.6040D-08 -V/T = 2.0050
S**2 = 0.0000

Dipole moment (field-independent basis, Debye):

```
    X=     2.4650    Y=     0.9567    Z=     0.0000  Tot=     2.6442

1                     2                     3
                     A'                    A"                    A'
 Frequencies -- -1048.1280              480.9560              767.3256


Zero-point correction=                           0.056058 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.581668
Sum of electronic and thermal Enthalpies=            -154.577138 (95.3)
Sum of electronic and thermal Free Energies=         -154.606682

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  37.427             12.100            62.180


Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.278022   -0.393007    0.729650
    2          6             0       -1.034693   -0.287374    0.000000
    3          6             0        0.278022    0.867432    0.000000
    4          6             0        0.278022   -0.393007   -0.729650
    5          1             0        0.807510    1.800747    0.000000
    6          1             0        0.689880   -0.839017   -1.611426
    7          1             0        0.689880   -0.839017    1.611426
    8          1             0       -0.983505    1.113030    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     14.9374974     13.3601078     12.6290171
```

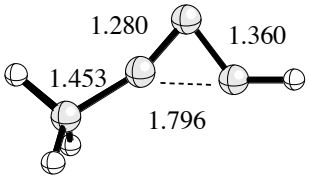


TS(10,4)

```
SCF Done:  E(RB+HF-LYP) =  -154.637818312     A.U. after   10 cycles
             Convg  =    0.9210D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                     A                     A                     A
 Frequencies --  -995.1829              139.1985              165.9388

Zero-point correction=                           0.056663 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.581155 (96.2)
 Sum of electronic and thermal Energies=             -154.576335
 Sum of electronic and thermal Enthalpies=           -154.575391 (96.4)
 Sum of electronic and thermal Free Energies=        -154.607914

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.581             14.266            68.449

Dipole moment (field-independent basis, Debye):
    X=     2.0386    Y=     0.0027    Z=    -0.5157  Tot=     2.1028

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.563762   -0.146731    0.039206
    2          1             0        2.110733    0.771859    0.270026
    3          1             0        2.078307   -0.682928   -0.755746
    4          1             0        1.558454   -0.769148    0.941720
    5          6             0        0.181544    0.186364   -0.262617
```

6	6	0	-0.920751	0.734167	0.088388
7	6	0	-1.411556	-0.532441	0.149014
8	1	0	-2.225484	-0.767937	-0.539949

Rotational constants (GHZ): 32.0502556 6.0962090 5.4522786



TS(10,DP1)

SCF Done: E(RB+HF-LYP) = -154.629079117 A.U. after 11 cycles
Convg = 0.3253D-08 -V/T = 2.0051
S**2 = 0.0000

1	2	3
A	A	A
Frequencies -- -1505.8156	169.6863	246.5532

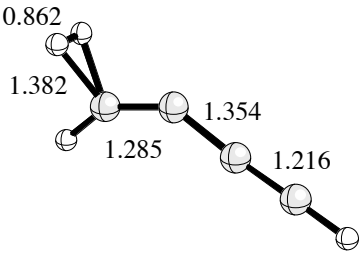
Zero-point correction= 0.050208 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.578871 (97.6)
Sum of electronic and thermal Energies= -154.573657
Sum of electronic and thermal Enthalpies= -154.572713 (98.1)
Sum of electronic and thermal Free Energies= -154.605275

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	34.778	17.250	68.533

Dipole moment (field-independent basis, Debye):
X= 2.5097 Y= 0.7893 Z= 0.0011 Tot= 2.6309

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.631644	0.267922	0.000038
2	6	0	0.500021	-0.341026	-0.000336
3	6	0	-0.827424	-0.072903	-0.000205
4	6	0	-2.033525	0.080012	0.000172
5	1	0	-3.082226	0.237126	0.000537
6	1	0	2.670601	-0.534283	-0.430581
7	1	0	2.669632	-0.535564	0.431873
8	1	0	2.117698	1.228690	0.000159

Rotational constants (GHZ): 102.7885249 4.1673630 4.0289235

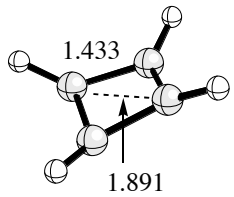


TS(12,5)

SCF Done: E(UB+HF-LYP) = -154.689232857 A.U. after 28 cycles
Convg = 0.6345D-08 -V/T = 2.0050
S**2 = 0.4927

1	2	3
A1	B2	A1

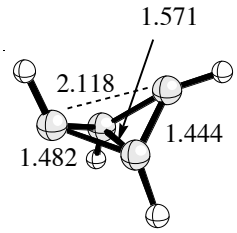
```
 Frequencies --  -732.7786               268.3069               622.7727

Zero-point correction=                           0.060739 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.628494
 Sum of electronic and thermal Energies=             -154.624720
 Sum of electronic and thermal Enthalpies=           -154.623776 (66.0)
 Sum of electronic and thermal Free Energies=        -154.653222

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.482             12.006             61.976

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=     1.3892  Tot=     1.3892

Largest concise Abelian subgroup C2V     NOp   4
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.000000    1.064059   -0.131321
    2          6             0        0.000000   -1.064059   -0.131321
    3          6             0       -0.945266    0.000000    0.037494
    4          6             0        0.945266    0.000000    0.037494
    5          1             0        0.000000   -2.108767    0.117621
    6          1             0       -1.950873    0.000000    0.445345
    7          1             0        1.950873    0.000000    0.445345
    8          1             0        0.000000    2.108767    0.117621
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     16.8643197     13.6633140      7.7449412
```



TS(12,15)

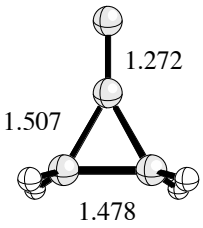
```
SCF Done:  E(UB+HF-LYP) =  -154.646369550     A.U. after   26 cycles
             Convg  =    0.6294D-08             -V/T =  2.0050
             S**2   =   0.9042
1                    2                     3
                    A'                    A'                    A'
 Frequencies --  -708.1443               488.3547               690.4034

Zero-point correction=                           0.057175 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.589194
 Sum of electronic and thermal Energies=             -154.585530
 Sum of electronic and thermal Enthalpies=           -154.584585 (90.6)
 Sum of electronic and thermal Free Energies=        -154.614338

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.178             12.556             62.619

Dipole moment (field-independent basis, Debye):
    X=     0.4366    Y=     1.0889    Z=     0.0000  Tot=     1.1731

Largest concise Abelian subgroup CS      NOp   2
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.261064   -1.120918    0.000000
    2          6             0        0.261064    0.135853    0.785338
    3          6             0        0.261064    0.135853   -0.785338
    4          6             0       -0.806925    0.707673    0.000000
    5          1             0       -1.383057    1.616207    0.000000
    6          1             0        1.019691    0.558202   -1.424276
    7          1             0        1.019691    0.558202    1.424276
```

```
    8          1             0       -0.513928   -1.883374    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     17.7404116     11.7780883      9.6810358
```



TS(13,13')

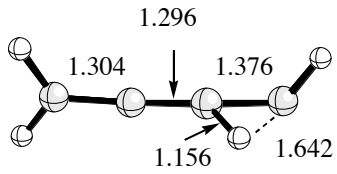
```
SCF Done:  E(RB+HF-LYP) =  -154.704393382     A.U. after   11 cycles
             Convg  =    0.4831D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                    B2                   B1                   A1
 Frequencies --   -56.5702              244.4176              742.9769

Zero-point correction=                           0.060442 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.643951 (56.8)
 Sum of electronic and thermal Energies=              -154.640175
 Sum of electronic and thermal Enthalpies=            -154.639231 (56.3)
 Sum of electronic and thermal Free Energies=         -154.668943

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.298             11.883             62.536

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=    -4.3375  Tot=     4.3375

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.000000    0.000000    0.511499
    2          6             0        0.000000    0.000000    1.783994
    3          6             0        0.000000    0.738908   -0.801980
    4          6             0        0.000000   -0.738908   -0.801980
    5          1             0        0.916405    1.262820   -1.037299
    6          1             0       -0.916405    1.262820   -1.037299
    7          1             0       -0.916405   -1.262820   -1.037299
    8          1             0        0.916405   -1.262820   -1.037299
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     22.0517237      7.8762763      6.2927237
```



TS(14b,2)

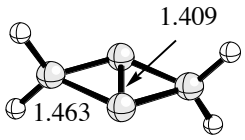
```
SCF Done:  E(RB+HF-LYP) =  -154.669723574     A.U. after    9 cycles
             Convg  =    0.9866D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -452.2168              197.5253              242.9590
```

```
Zero-point correction=                           0.054439 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.615284 (74.8)
Sum of electronic and thermal Enthalpies=            -154.609659(74.9)
 Sum of electronic and thermal Free Energies=         -154.641356

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  37.098             15.047             66.711

Dipole moment (field-independent basis, Debye):
    X=    -1.0710    Y=     1.6848    Z=     0.2939  Tot=     2.0179

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.898744   -0.001580   -0.067056
    2          6             0       -0.599901   -0.033028    0.040368
    3          6             0        0.690319    0.071038    0.106433
    4          6             0        2.006988   -0.228495   -0.156231
    5          1             0        2.571368    0.686786   -0.393367
    6          1             0       -2.507255   -0.874853    0.147908
    7          1             0       -2.430444    0.891376   -0.381993
    8          1             0        1.174360    0.449082    1.086367
 ---------------------------------------------------------------------
```



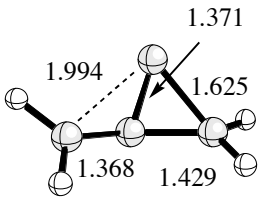
TS(20,20')

```
SCF Done:  E(UB+HF-LYP) =  -154.666245557     A.U. after    1 cycles
             Convg  =    0.1819D-08             -V/T =  2.0050
             S**2   =   0.0000

Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000

1                     2                     3
                     B1U                   B2U                   B3G
 Frequencies --  -383.0033              469.5742              820.6017

Zero-point correction=                           0.061085 (Hartree/Particle)
Thermal correction to Enthalpy=                  0.065412
Sum of electronic and zero-point Energies=           -154.605160 (81.1)
 Sum of electronic and thermal Energies=             -154.601778
 Sum of electronic and thermal Enthalpies=           -154.600834 (80.4)
 Sum of electronic and thermal Free Energies=        -154.628870

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  40.454             10.427             59.006

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.000000    0.704646    0.000000
    2          6             0        1.282522    0.000000    0.000000
    3          6             0        0.000000   -0.704646    0.000000
    4          6             0       -1.282522    0.000000    0.000000
    5          1             0        1.889161    0.000000    0.908624
    6          1             0        1.889161    0.000000   -0.908624
    7          1             0       -1.889161    0.000000    0.908624
    8          1             0       -1.889161    0.000000   -0.908624
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     33.1507875      8.8364792      7.6827805
```



TS(20,28)

```
CF Done:  E(RB+HF-LYP) =  -154.668915349     A.U. after   10 cycles
             Convg  =    0.9110D-08             -V/T =  2.0050
             S**2   =   0.0000
1                    2                    3
                     A                    A                    A
 Frequencies --  -309.2923               371.2975               472.7239

Zero-point correction=                           0.059760 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.609155
 Sum of electronic and thermal Energies=             -154.605404
 Sum of electronic and thermal Enthalpies=           -154.604459 (78.15)
 Sum of electronic and thermal Free Energies=        -154.634543

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   39.854             12.089            63.315

Dipole moment (field-independent basis, Debye):
    X=    -0.7470    Y=    -2.2299    Z=    -0.3174  Tot=     2.3730

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.251638    0.963325    0.255299
    2          6             0       -1.333749   -0.229296    0.051934
    3          6             0       -0.087688   -0.127918   -0.502905
    4          6             0        1.209019   -0.334882    0.059691
    5          1             0       -2.070034    0.527780   -0.169338
    6          1             0       -1.642477   -1.065603    0.674948
    7          1             0        2.055104   -0.056400   -0.553923
    8          1             0        1.422082   -1.033153    0.864202
 ---------------------------------------------------------------------
```



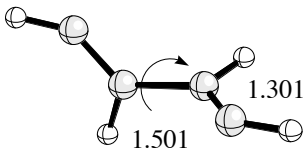
TS(22,24)

```
SCF Done:  E(UB+HF-LYP) =  -154.666477274     A.U. after    9 cycles
             Convg  =    0.5205D-08             -V/T =  2.0049
             S**2   =   0.9979

1                    2                    3
                     A                    A                    B
 Frequencies --  -167.9029               332.2358               377.8848

Zero-point correction=                           0.055897 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.610580 (77.7)
Sum of electronic and thermal Enthalpies=            -154.605424 (77.5)
Sum of electronic and thermal Free Energies=         -154.635787

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   37.719             14.421            63.905
```

Dipole moment (field-independent basis, Debye):
X= 0.0000 Y= 0.0000 Z= 0.8015 Tot= 0.8015

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.550072	1.605229	-0.387386
2	1	0	1.175206	2.466497	-0.551054
3	6	0	0.547344	0.513785	0.319882
4	6	0	-0.547344	-0.513785	0.319882
5	1	0	-1.379662	-0.305645	0.998300
6	6	0	-0.550072	-1.605229	-0.387386
7	1	0	-1.175206	-2.466497	-0.551054
8	1	0	1.379662	0.305645	0.998300



TS(22,DP2)

SCF Done: E(UB+HF-LYP) = -154.666561494 A.U. after 12 cycles
Convg = 0.7349D-08 -V/T = 2.0050
S**2 = 0.3837

1 A -879.9657 0.8002 0.0013
Zero-point correction= 0.053872 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.612690 (76.4)
Sum of electronic and thermal Enthalpies= -154.606597 (76.8)
Sum of electronic and thermal Free Energies= -154.639079

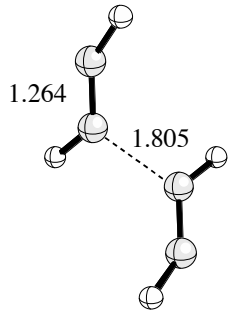
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	37.036	16.978	68.364

Dipole moment (field-independent basis, Debye):
X= 0.0000 Y= 0.0000 Z= 0.1978 Tot= 0.1978

Input orientation:

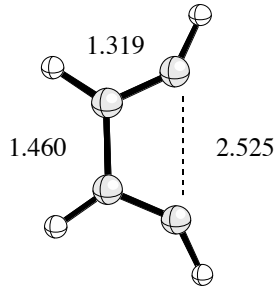
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745666	1.590450	0.323229
2	1	0	-0.251210	2.242605	1.019978
3	6	0	-0.745666	0.508539	-0.329661
4	6	0	0.745666	-0.508539	-0.329661
5	1	0	1.442098	-0.001281	-0.981381
6	6	0	0.745666	-1.590450	0.323229
7	1	0	0.251210	-2.242605	1.019978
8	1	0	-1.442098	0.001281	-0.981381

1	2	3
	A	A	A
Frequencies --	-879.9657	101.0156	285.3969



TS(24,5)

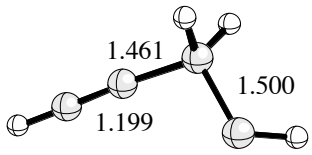
```
SCF Done:  E(UB+HF-LYP) =  -154.667292281     a.u. after   16 cycles
            Convg  =    0.4509D-07                    82 Fock formations.
              S**2 =  0.7853                  -V/T =  2.0049

 Annihilation of the first spin contaminant:
 S**2 before annihilation     0.7853,   after     0.2192

1                     2                     3
                     A'                    A"                    A"
 Frequencies --  -342.1590               243.9855              546.5309

Zero-point correction=                           0.056642 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -154.610650 (77.7)
 Sum of electronic and thermal Energies=            -154.606534
 Sum of electronic and thermal Enthalpies=          -154.605590 (77.4)
 Sum of electronic and thermal Free Energies=       -154.636502

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.127             13.844             65.060

Dipole moment (field-independent basis, Debye):
    X=    -0.6387    Y=     0.5003    Z=     0.0000  Tot=     0.8114

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.278714   -1.385425    0.000000
    2          1             0       -0.502015   -2.439596    0.000000
    3          6             0       -0.900662   -0.221943    0.000000
    4          6             0        0.000000    0.927603    0.000000
    5          1             0       -0.355697    1.957402    0.000000
    6          6             0        1.278501    0.602090    0.000000
    7          1             0        2.248621    1.071169    0.000000
    8          1             0       -1.985657   -0.122925    0.000000
 ---------------------------------------------------------------------
```



TS(27a27b)

```
SCF Done:  E(RB+HF-LYP) =  -154.655434178     A.U. after    9 cycles
            Convg  =    0.7763D-08             -V/T =  2.0050
            S**2   =   0.0000

1                     2                     3
                     A                     A                     A
```

```
 Frequencies --  -407.4076               240.4401               323.6679

Zero-point correction=                           0.056626 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.598808 (85.0)
 Sum of electronic and thermal Energies=             -154.594427
 Sum of electronic and thermal Enthalpies=           -154.593483 (85.0)
 Sum of electronic and thermal Free Energies=        -154.624949

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  38.283             14.434             66.225

Dipole moment (field-independent basis, Debye):
    X=    -0.0193    Y=     1.7005    Z=     1.1472  Tot=     2.0514

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.807486   -0.221719    0.023364
    2          1             0        2.818916   -0.542819    0.041324
    3          6             0        0.671090    0.158296   -0.013046
    4          6             0       -0.731032    0.569862    0.007037
    5          1             0       -0.930843    1.150277   -0.907179
    6          6             0       -1.539842   -0.685145   -0.141178
    7          1             0       -2.211221   -0.750291    0.737680
    8          1             0       -0.923065    1.215069    0.871111
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     30.8366723      5.2355824      4.6688866
```

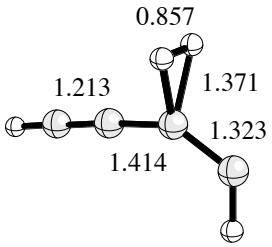


$$\tau(CC(H_2)CH) = 122.5°$$

TS(27a,DP1)

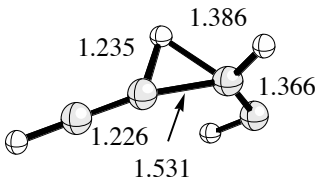
```
SCF Done:  E(RB+HF-LYP) =  -154.612044321     A.U. after    8 cycles
             Convg  =    0.7560D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies -- -1349.0251               234.0588               291.2863

Zero-point correction=                           0.051158 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.560887 (108.9)
Sum of electronic and thermal Enthalpies=            -154.555255  109.0)
Sum of electronic and thermal Free Energies=         -154.587038

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  35.043             16.094             66.891

Dipole moment (field-independent basis, Debye):
    X=    -2.4221    Y=     1.1681    Z=     0.0000  Tot=     2.6890

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.910216   -0.165150   -0.000003
    2          1             0        2.956354   -0.377944    0.000045
    3          6             0        0.716494    0.048849   -0.000007
    4          6             0       -0.682254    0.256675   -0.000007
    5          1             0       -0.853060    1.547237    0.428633
    6          6             0       -1.856908   -0.352372    0.000015
    7          1             0       -0.853087    1.547212   -0.428633
```

8	1	0	-1.775497	-1.444517	-0.000033



TS(27a,DP2)

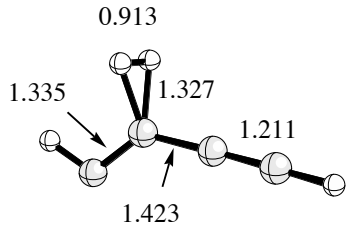
```
SCF Done:  E(RB+HF-LYP) =  -154.606605834     A.U. after    1 cycles
             Convg  =    0.1855D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                      A                     A                     A
 Frequencies -- -1225.8027              202.1943              375.2883

Zero-point correction=                           0.052753 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.553852 (113.3)
Sum of electronic and thermal Enthalpies=            -154.548225 (113.4)
Sum of electronic and thermal Free Energies=         -154.580091

                      E (Thermal)             CV                S
                       KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                    36.042             15.921             67.067

Dipole moment (field-independent basis, Debye):
    X=     3.5158    Y=     0.5504    Z=     1.2628  Tot=     3.7760

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.844468   -0.200436   -0.071248
    2          1             0        2.854246   -0.520085   -0.209272
    3          6             0        0.675794    0.143884    0.068659
    4          6             0       -0.808945    0.496532   -0.049798
    5          1             0        0.017758    0.466886    1.062847
    6          6             0       -1.788058   -0.455018   -0.103142
    7          1             0       -1.479285   -1.413236    0.339126
    8          1             0       -0.932271    1.556663   -0.259524
 ---------------------------------------------------------------------
```



TS(27b,DP1)

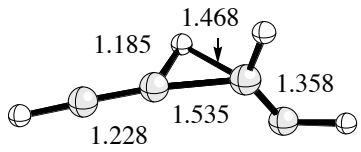
```
SCF Done:  E(RB+HF-LYP) =  -154.613366974     A.U. after    8 cycles
             Convg  =    0.7787D-08             -V/T =  2.0050
             S**2   =   0.0000

1                     2                     3
                      A                     A                     A
 Frequencies -- -1527.8361              234.7392              290.3532

Zero-point correction=                           0.050486 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.562881 (107.6)
Sum of electronic and thermal Enthalpies=            -154.557237 (107.8)
```

```
Sum of electronic and thermal Free Energies=         -154.589004

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  34.630             16.110             66.860

Dipole moment (field-independent basis, Debye):
    X=     0.6979    Y=     3.2835    Z=     0.0004  Tot=     3.3568

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.928805   -0.142545   -0.000115
    2          1             0        2.980433   -0.325149    0.000704
    3          6             0        0.730671    0.030622   -0.000086
    4          6             0       -0.676136    0.244130    0.000019
    5          1             0       -0.859476    1.476222   -0.456159
    6          6             0       -1.741631   -0.560465    0.000036
    7          1             0       -2.711692   -0.057296   -0.000125
    8          1             0       -0.859515    1.475771    0.456457
 ---------------------------------------------------------------------
```



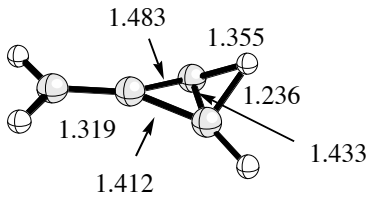
TS(27b,DP2)

```
SCF Done:  E(RB+HF-LYP) =  -154.603671316     A.U. after    9 cycles
             Convg  =    0.8871D-08             -V/T =  2.0050
             S**2   =    0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -974.5137              207.1270             384.0212

Zero-point correction=                           0.052539 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.551132 (115.0)
Sum of electronic and thermal Enthalpies=            -154.545518 (115.1)
Sum of electronic and thermal Free Energies=         -154.577277

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  35.899             16.041             66.841


Dipole moment (field-independent basis, Debye):
    X=     2.5329    Y=     2.3135    Z=    -0.0479  Tot=     3.4308

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.892280   -0.163909   -0.085868
    2          1             0        2.922398   -0.404285   -0.234603
    3          6             0        0.698307    0.074174    0.077614
    4          6             0       -1.720007   -0.542898    0.026640
    5          1             0       -2.673117   -0.179119   -0.389749
    6          6             0       -0.785466    0.438259   -0.066315
    7          1             0       -0.856967    1.524318   -0.175503
    8          1             0        0.097005    0.225334    1.087429
 ---------------------------------------------------------------------
```



TS(28,3)

```
SCF Done:  E(RB+HF-LYP) =  -154.654345775     A.U. after   11 cycles
             Convg  =    0.3213D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -933.3151              344.5096              381.8267

Zero-point vibrational energy     146300.0 (Joules/Mol)
                                   34.96653 (Kcal/Mol)
Sum of electronic and zero-point Energies=           -154.598623
 Sum of electronic and thermal Energies=             -154.594595
 Sum of electronic and thermal Enthalpies=           -154.593651 (84.9)
 Sum of electronic and thermal Free Energies=        -154.624236

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  37.494             13.438             64.371

Dipole moment (field-independent basis, Debye):
    X=    -0.6831    Y=     2.4837    Z=     0.4635  Tot=     2.6172

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.252960   -0.001047    0.066773
    2          6             0        1.568819    0.057432    0.003094
    3          6             0       -1.036051    0.566502   -0.031708
    4          6             0       -0.940574   -0.861150   -0.117525
    5          1             0       -1.671387    1.413525   -0.247532
    6          1             0       -1.650098   -0.134914    0.779802
    7          1             0        2.093824    1.001261   -0.050064
    8          1             0        2.156739   -0.850292   -0.006015
 ---------------------------------------------------------------------
```



TS(29,12)

```
SCF Done:  E(UB+HF-LYP) =  -154.646995337     A.U. after   18 cycles
             Convg  =    0.9094D-08             -V/T =  2.0050
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies --  -186.2852              439.9399              586.4572

Zero-point correction=                           0.057821 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -154.589174
 Sum of electronic and thermal Energies=             -154.585415
 Sum of electronic and thermal Enthalpies=           -154.584471 (90.7)
 Sum of electronic and thermal Free Energies=        -154.614546
```

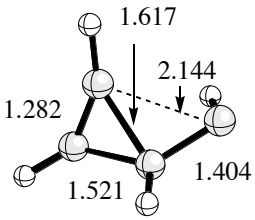
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	38.642	12.731	63.299

Dipole moment (field-independent basis, Debye):
X= -4.1374 Y= -0.1448 Z= -0.1667 Tot= 4.1433

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.459376	0.101048	-0.165124
2	1	0	1.261923	0.530699	-1.157435
3	6	0	0.319238	-0.602661	0.253394
4	1	0	0.338909	-1.182394	1.175120
5	6	0	-1.067566	-0.305095	-0.295788
6	6	0	-0.548594	0.760838	0.192933
7	1	0	-0.598348	1.728499	0.653675
8	1	0	-1.977214	-0.801585	-0.583844

Rotational constants (GHZ): 21.0728667 8.9944647 7.4339889



TS(29,DP2)

SCF Done: E(RB+HF-LYP) = -154.643499363 A.U. after 10 cycles
Convg = 0.5075D-08 -V/T = 2.0050
S**2 = 0.0000

1	2	3
	A	A	A
Frequencies --	-481.7830	218.2615	417.8647

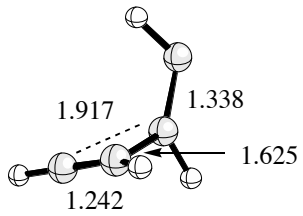
Zero-point correction= 0.055505 (Hartree/Particle)
Sum of electronic and zero-point Energies= -154.587994 (91.9)
Sum of electronic and thermal Enthalpies= -154.582535 (91.9)
Sum of electronic and thermal Free Energies= -154.614061

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	37.663	15.386	66.353

Dipole moment (field-independent basis, Debye):
X= -4.1547 Y= -0.0168 Z= -0.2722 Tot= 4.1637

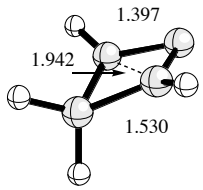
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.524670	0.008561	0.512251
2	6	0	1.618702	-0.109049	-0.248275
3	6	0	-1.205183	-0.534936	-0.109705
4	6	0	-0.824494	0.647447	-0.128617
5	1	0	-1.564495	-1.536555	-0.108335
6	1	0	-1.012752	1.686423	-0.320072
7	1	0	1.423763	-0.235703	-1.316444
8	1	0	0.471318	0.013698	1.590926



TS (33,9)

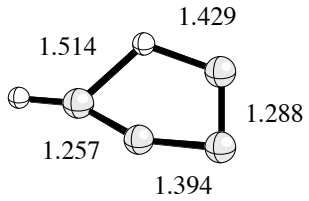
```
SCF Done:  E(UB+HF-LYP) =  -154.670784362     A.U. after    1 cycles
             Convg  =    0.8454D-10             -V/T =  2.0049
             S**2   =   0.4699

Dipole moment (field-independent basis, Debye):
    X=    -2.5770    Y=    -1.0440    Z=    -0.5072  Tot=     2.8263

1                    2                    3
                     A                    A                    A
 Frequencies -- -1627.9532               434.2007              669.2062

Zero-point correction=                          0.058858 (Hartree/Particle)
Thermal correction to Enthalpy=                 0.063378
Sum of electronic and zero-point Energies=          -154.611926 (76.9)
 Sum of electronic and thermal Energies=            -154.608350
 Sum of electronic and thermal Enthalpies=          -154.607406 (76.3)
 Sum of electronic and thermal Free Energies=       -154.637159

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  39.178             11.637            62.621

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.959115   -0.320415    0.053020
    2          6             0       -0.168874    0.967333   -0.069667
    3          6             0        0.482843   -0.861785   -0.022543
    4          6             0        1.096769    0.365974    0.111558
    5          1             0       -1.450091   -0.472346    1.013183
    6          1             0       -1.634027   -0.608188   -0.758970
    7          1             0        0.841899   -1.812162   -0.402546
    8          1             0       -0.467523    1.986049   -0.285869
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     15.4083394     13.8571617      7.7663909
```



TS(DP3,DP1)

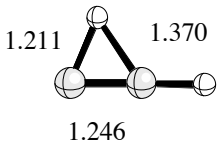
```
SCF Done:  E(UB+HF-LYP) =  -153.364367727     A.U. after   10 cycles
             Convg  =    0.2304D-08             -V/T =  2.0047
             S**2   =   0.0000

1                    2                    3
                     A                    A                    A
 Frequencies -- -1637.8004               373.3067              414.6669

Zero-point correction=                          0.030006 (Hartree/Particle)
Sum of electronic and zero-point Energies=          -153.334361
 Sum of electronic and thermal Energies=            -153.330346
```

```
 Sum of electronic and thermal Enthalpies=           -153.329402 (146.2)
 Sum of electronic and thermal Free Energies=        -153.359667

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  21.349             12.791            63.697

Dipole moment (field-independent basis, Debye):
    X=    -2.7274    Y=     0.5936    Z=     0.0005  Tot=     2.7912

Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.017005    0.729625    0.000045
    2          1             0       -0.337830    1.182993   -0.000054
    3          6             0        1.115503   -0.554801   -0.000080
    4          6             0       -0.277099   -0.491170    0.000125
    5          6             0       -1.389883    0.093841   -0.000116
    6          1             0       -2.455328    0.152036    0.000212
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     34.9386614      8.7891733      7.0225740
```



TS(DP4,DP2)

```
SCF Done:  E(RB+HF-LYP) =  -77.2871651474     A.U. after    7 cycles
             Convg  =    0.1519E-08             -V/T =  2.0049
             S**2   =   0.0000

1                    2                    3
                    A'                   A"                   A'
 Frequencies --  -852.9380              586.0421             915.5729

Zero-point correction=                           0.021017 (Hartree/Particle)
Sum of electronic and zero-point Energies=           -77.266148 (83.4)
 Sum of electronic and thermal Energies=             -77.263096
 Sum of electronic and thermal Enthalpies=           -77.262152 (84.8)
 Sum of electronic and thermal Free Energies=        -77.287409

                       E                CV                S
                    KCAL/MOL       CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 15.104             7.524            53.157

Dipole moment (Debye):
    X=    -0.8789    Y=     3.0284    Z=     0.0000  Tot=     3.1534

Standard orientation:
 ---------------------------------------------------------------
 Center     Atomic             Coordinates (Angstroms)
 Number     Number            X           Y           Z
 ---------------------------------------------------------------
    1          6          0.077923   -0.732050    0.000000
    2          6          0.077923    0.513772    0.000000
    3          1         -1.042767   -0.273827    0.000000
    4          1          0.107697    1.583499    0.000000
 ---------------------------------------------------------------
 Rotational constants (GHZ):    417.0272393     41.6141519     37.8383530
```


1.211
1.370
1.246