

Supporting Information

A DFT study of endocyclic allenes - unprecedentedly superbasic hydrocarbons

Davor Margetić,* and Ivana Antol

Ruđer Bošković Institute, Bijenička cesta 54, HR-10002 Zagreb, Croatia

1. Computational details

Computational Details

All geometrical optimizations were carried out employing B3LYP hybrid functional DFT method (Becke's 3 parameter functional with the non-local correlation provided by the expression of Lee *et al.*)¹ as well as M052X² and M062X³ hybrid functionals of Truhlar and Zhao employing 6-31G* basis set. Calculations were performed using *Gaussian03* suite of programs,⁴ implemented on dual core Opteron 240 personal computer under Linux operating system and computer cluster Isabella at the Computing center of the University of Zagreb (Isabella computer cluster (24 dual processor HP ProLiant BLP20p nodes with Intel Xeon 2.8 GHz, 32 dual processor Dell 1850 1U nodes with Intel Xeon 3.4 GHz and 24 dual processor Pyramid GX28 nodes with AMD Opteron 248). Harmonic vibration frequencies were calculated for all localized stationary structures to verify minima by no possession of imaginary vibrations. Single point calculations were conducted using B3LYP/6-311+G**//B3LYP//6-31G* method, and the gas phase basicity (GB) were calculated as the Gibbs free energy change of the protonation reaction. Throughout the manuscript, B3LYP⁵ denotes PA calculated at B3LYP/6-31G*+ E_{vib} (B3LYP/6-31G*), while B3LYP(2)⁶ denotes the PA obtained at the B3LYP/6-311+G**//B3LYP/6-31G*+ E_{vib} (B3LYP/6-31G*) level. Likewise, notation for M052X, M052X(2), M062X and M062X(2) was applied. Hybridization, Wiberg and BOAO bond orders were obtained from NBO analysis incorporated within *Gaussian03* program using pop=nboread keyword.

Proton affinity of allenes in the gas phase ($\text{PA}_{\text{B3LYP}(2)}$) was calculated using the following equations:⁶

$$\text{PA}(\text{B}) = \Delta E_{\text{el}} + \Delta \text{ZPVE}_{\text{B3LYP}} \quad (1)$$

$$\Delta E_{\text{el}} = E(\text{B})_{\text{B3LYP}(2)} - E(\text{BH}^+)_{\text{B3LYP}(2)} \quad (2)$$

$$\Delta \text{ZPVE}_{\text{B3LYP}} = \text{ZPVE}(\text{B})_{\text{B3LYP}} - \text{ZPVE}(\text{BH}^+)_{\text{B3LYP}} \quad (3)$$

Here B3LYP denotes B3LYP/6-31G* level; while B3LYP(2) is B3LYP/6-311+G**//B3LYP/6-31G* model. Similarly, PA_{M052X(2)} and PA_{M062X(2)} were obtained.

Gas phase basicities (GB) of allenes are defined as a negative value of the free energy change for the protonation reaction.

The solvent effect in acetonitrile was estimated by employing the polarized continuum model at IPCM/B3LYP/6-311+G** //B3LYP//6-31G* level.⁷ The molecular surface determining a cavity within a solvent is obtained by the isodensity shell of 0.0004eB⁻³, thus giving rise to the isodensity polarized continuum model (IPCM)⁸ utilizing dielectric constant for acetonitrile $\epsilon = 36.64$. Estimation of PA and pK_a values in acetonitrile was achieved by using the equations derived for guanidines:⁹

$$pK_a = 0.4953PA(B_{MeCN}) - 119.7 \text{ units} \quad (4)$$

$$PA(B_{MeCN}) = \Delta E_{el MeCN} + \Delta ZPVE_{B3LYP} \quad (5)$$

$$\Delta E_{el MeCN} = E(B)_{MeCN} - E(BH^+)_{MeCN} \quad (6)$$

$$\Delta ZPVE_{B3LYP} = ZPVE(B)_{B3LYP} - ZPVE(BH^+)_{B3LYP} \quad (7)$$

In these equations MeCN denotes IPCM/B3LYP/6-311+G**//B3LYP/6-31G* model and B3LYP denotes B3LYP/6-31G* method, hence $PA_{MeCN} = IPCM/6-311+G^{**}/B3LYP/6-31G^* + E_{vib}(B3LYP/6-31G^*)$.¹⁰

Table SI-1. Geometrical parameters (B3LYP/6-31G*)

Base	C ₁ =C ₂ Distance /Å	C ₁ =C ₂ =C ₃ Angle / °	C ₁ =C ₂ =C ₃ -C ₄ Angle / °	C ₁ / C ₂ / C ₃ p hybridization ^a	Bond order Wiberg	Bond order BOAO
1	1.330	145.9	27.0	1.80 / 1.09	1.8091	1.3521
2	1.332	145.2	25.8/26.9	1.80 / 1.09 / 1.80	1.8023/ 1.8004	1.3452/ 1.3473
3	1.332	144.9	26.4/26.5	1.80 / 1.09 / 1.80	1.8027/ 1.7964	1.3454/ 1.3458
4	1.337/1.347	139.4	27.4/23.2	1.68 / 1.15 / 1.76	1.6483/1.8037	1.2965/ 1.3387
5	1.336/1.346	139.5	23.7/27.2	1.68 / 1.15 / 1.76	1.6545/ 1.8059	1.2994/ 1.3401
6	1.334/1.338	144.0	26.6/25.3	1.81 / 1.10 / 1.79	1.7654/ 1.7998	1.3279/ 1.3442
7	1.331/1.337	143.5	25.8/27.8	1.80 / 1.10 / 1.82	1.8081/ 1.7545	1.3491/ 1.3262
8	1.351/1.337	138.3	23.2/25.7	1.68 / 1.16 / 1.74	1.6302/ 1.7902	1.2871/ 1.3341
9	1.365/1.350	138.8	24.3/24.9	1.70 / 1.16 / 1.74	1.6243/ 1.8063	1.2833/ 1.3420
10	1.363	130.8	21.4/21.5	1.67 / 1.22 / 1.67	1.6001/ 1.6000	1.2630/ 1.2630
11	1.362/1.365	131.9	20.6/21.4	1.66 / 1.23 / 1.67	1.6046/ 1.5824	1.2677/ 1.255
12	1.359	131.2	20.9/20.2	1.64 / 1.20 / 1.62	1.6340/ 1.657	1.2768 /1.2890
13	1.353	135.1	27.9/28.1	1.62 / 1.21 / 1.62	1.6141/ 1.6138	1.2998/ 1.2996
14	1.349/1.355	137.8	19.3/33.9	1.68 / 1.08 / 1.65	1.6533/ 1.6301	1.3111/ 1.3017
15	1.375	128.7	19.7/23.8	1.69 / 1.29 / 1.70	1.5105/ 1.5075	1.2312/1.2297
16	1.333/1.335	146.4	17.8/19.4	1.79 / 1.06 / 1.80	1.6577/ 1.6452	1.3183/1.3113
17	1.336/1.338	144.5	18.0/19.8	1.78 / 1.08 / 1.79	1.6541/ 1.6420	1.3119/ 1.3051
18	1.339/1.343	142.6	18.3/19.9	1.77 / 1.09 / 1.78	1.6555/ 1.6285	1.3094/1.2956
19	1.349/1.352	136.1	18.4/20.6	1.68 / 1.16 / 1.69	1.6302/ 1.6209	1.2798/ 0.9349

^a 1.80 denotes sp^{1.80}

Table SI-2. Gas phase proton affinities, basicities (kcal mol⁻¹) and pK_a values

Base	B3LYP					M052X				M062X			
	PA _B ^a	PA _{B(2)} ^b	GB _B ^c	PA _{MeCN}	pK _a	PA _{M05(2)} ^d	GB _{M05}	PA _{MeCN}	pK _a	PA _{M06(2)} ^e	GB _{M06}	PA _{MeCN}	pK _a
1	263.9	262.5	257.8	305.9	31.8	251.2	250.4	299.4	28.6	249.2	248.5	297.7	27.7
2	276.2	269.3	270.0	312.5	35.0	263.1	262.2	305.7	31.7	261.2	260.4	304.1	30.9
3	279.9	273.3	273.8	311.5	34.6	266.6	265.4	304.4	31.1	265.0	264.0	303.1	30.4
4	281.3	274.4	275.1	317.2	37.4	269.6	268.9	312.2	34.9	267.6	266.9	310.5	34.1
5	284.4	277.6	278.3	315.4	36.5	272.4	271.5	310.0	33.9	271.3	269.9	308.6	33.1
6	285.5	278.7	279.3	317.7	37.7	272.7	271.7	311.3	34.5	270.8	269.9	317.4	37.5
7	290.5	284.0	284.1	316.3	37.0	278.0	276.3	314.3	36.0	276.7	275.1	308.5	33.1
8	290.3	287.7	284.1	317.7	37.7	279.5	279.4	318.3	38.0	277.3	275.9	316.5	37.1
9	294.5	288.4	288.6	327.6	42.6	284.2	282.7	320.1	38.8	282.8	281.6	314.4	36.0
10	293.6	286.2	287.3	323.5	40.5	283.7	283.5	321.1	39.3	281.9	281.2	319.7	38.6
11	299.4	291.9	293.1	326.2	41.8	290.2	289.6	324.1	40.8	287.9	287.5	322.6	40.1
12	300.5	292.8	294.1	327.4	42.5	290.8	290.6	325.6	41.5	289.1	288.8	324.3	40.9
13	284.7	278.7	278.1	315.2	36.4	275.9	275.4	311.3	34.5	274.9	273.6	313.3	35.5
14	287.2	280.3	280.6	308.2	33.0	277.1	276.4	308.4	33.0	282.8	274.9	311.1	34.4
15	322.5	313.5	316.1	338.6	48.0	310.6	311.7	334.4	45.9	308.7	309.7	329.9	43.7
16	330.1	321.9	323.5	352.2	54.7	317.7	317.3	346.5	51.9	314.7	308.5	338.3	47.9
17	337.0	329.0	330.8	352.5	54.9	326.1	325.9	346.8	52.1	323.7	324.2	346.9	52.1
18	358.8	350.9	352.7	363.5	60.3	347.7	348.0			345.0	345.7		
19	327.4	318.5	320.7	334.7	46.1	302.9	302.8	319.0	38.3	301.4	301.5	337.8	47.6

^a PA_{B3LYP}: B3LYP/6-31G*+*E*_{vib}(B3LYP/6-31G*)⁸; ^b PA_{B3LYP(2)}: B3LYP/6-311+G**//B3LYP/6-31G*+ *E*_{vib}(B3LYP/6-31G*)⁹; ^c B3LYP/6-31G*; ^d PA_{M052X(2)}: M052X/6-311+G**//M052X/6-31G*+*E*_{vib}(M052X/6-31G*); ^e PA_{M062X(2)}: M062X/6-311+G**//M062X/6-31G*+*E*_{vib}(M062X/6-31G*)

2. Cartesian coordinates

B3LYP

Neutral

Allene 1 B3LYP/6-31G*

0	1			
C		1.294469	0.202020	0.695157
C		0.268624	0.182214	1.600695
C		-1.038023	-0.341047	1.225494
C		1.293502	-0.202061	-0.697405
C		-1.429149	-0.000261	0.001037
C		0.266194	-0.182626	-1.601175
C		-1.039467	0.341408	-1.223605
H		2.272248	0.494638	1.077814
H		0.471568	0.489010	2.627731
H		-1.588582	-1.015407	1.879953
H		2.270908	-0.493650	-1.081762
H		0.467410	-0.489558	-2.628515
H		-1.590451	1.017086	-1.876405

Allene 2 B3LYP/6-31G*

0	1			
C		0.37374500	-0.62317400	-0.09514400
C		0.53444400	0.75839100	-0.09982600
C		-0.57635700	1.64222100	-0.41342700
C		-0.80950300	-1.40932200	-0.31313200
C		-1.74555500	1.25424300	0.09209300
C		-2.11894400	-1.06408200	-0.08838700
C		-2.46481200	0.21435200	0.51286400
H		-0.45398500	2.48865000	-1.08864500
H		-0.62946500	-2.43487200	-0.63798300
H		-2.89081600	-1.80807800	-0.28869100
H		-3.21451800	0.27671300	1.30150800
C		1.94893300	1.08036200	0.10725900
H		2.33755700	2.09258200	0.15074900
C		2.66278500	-0.05865900	0.21571900
H		3.73349000	-0.13965300	0.36692700
C		1.74633900	-1.24416900	0.08396900
H		1.79533600	-1.90412700	0.96331700
H		2.01594600	-1.87219900	-0.77910300

Allene 3 B3LYP/6-31G*

0	1			
C		-0.76155100	-0.05084600	-0.16660800
C		-1.44423500	1.15097700	-0.02061500
C		-2.87212700	1.24744000	-0.27576700
C		-1.28254400	-1.34956800	-0.49401100
C		-3.57828800	0.20776400	0.16394700
C		-2.53731600	-1.85820100	-0.26239700
C		-3.53966000	-1.09158100	0.45876100
H		-3.29034000	2.06700400	-0.85968000
H		-0.56251800	-2.04586200	-0.92418400
H		-2.73752700	-2.88892000	-0.55816500
H		-4.15496000	-1.55717700	1.22844300
C		-0.48402600	2.21469000	0.27602600
H		-0.76126100	3.25086200	0.44186100
C		0.76177200	1.70467700	0.29630800
H		1.67180100	2.26327200	0.48300700
C		0.73900200	0.21775200	0.00013100
C		1.52519600	-0.10171700	-1.30730700
H		1.14181000	0.52325800	-2.12236800
H		1.32726200	-1.14544100	-1.58816200
C		1.33722000	-0.61589000	1.17224800
H		0.81910500	-0.35407800	2.10219600
H		1.12481000	-1.67708300	0.98258400
C		3.04333700	0.08134300	-1.15138200
H		3.54028700	-0.20540400	-2.08705300
H		3.27578200	1.14347300	-0.99295800
C		2.85485200	-0.43130500	1.32566900
H		3.21981200	-1.07785900	2.13394100
H		3.07513600	0.60020400	1.63432400
C		3.59728700	-0.74515900	0.01848400
H		3.48436600	-1.81511300	-0.21173500
H		4.67291600	-0.56338200	0.13704800

Allene 4 B3LYP/6-31G*

0	1			
C		-0.52974300	0.64907100	0.26065800
C		-0.44579800	-0.77769400	-0.02110500
C		0.69498000	-1.43872200	0.25402500
C		0.53359600	1.48964900	0.07427100
C		1.99865400	-1.18932400	0.41494900
C		1.87228900	1.14753600	-0.35115600
C		2.55110600	-0.04087100	-0.28403500
H		2.63169900	-1.77258900	1.08597400
H		3.56521600	-0.07468700	-0.68555300
C		-1.78281400	-1.20523700	-0.44471100
H		-2.01401300	-2.20166100	-0.80530000
C		-2.66859100	-0.21526800	-0.21735600
H		-3.74125200	-0.28194900	-0.36647300
C		-1.99767000	1.02144300	0.35465300
H		-2.33469100	1.20583000	1.38772400

H	-2.22131900	1.93535500	-0.21088100
H	0.33179100	2.55942400	0.12467400
H	2.42651400	1.98678400	-0.77132300

Allene 5 B3LYP/6-31G*

0 1			
C	-0.69020800	-0.16449400	0.03649100
C	-1.41558800	1.06533000	-0.25609400
C	-2.66741000	1.22444200	0.21131100
C	-1.32648900	-1.37524000	0.07789300
C	-3.70703900	0.48787800	0.61371800
C	-2.73476000	-1.65193900	-0.10989500
C	-3.83093300	-0.84701100	0.05128500
H	-0.70151500	-2.26540200	0.12914600
H	-4.40778200	0.82339900	1.38016300
H	-2.94195900	-2.68112900	-0.40357400
H	-4.81440100	-1.26992200	-0.16015100
C	-0.46903600	1.96195100	-0.92156700
H	-0.73886900	2.92272200	-1.34718600
C	0.77484000	1.45674700	-0.82017300
H	1.67355500	1.95618800	-1.16561800
C	0.81030400	0.10977600	-0.09202100
C	1.55774400	-0.98040200	-0.90277400
H	1.11974800	-1.05581700	-1.90517800
H	1.39943500	-1.95202400	-0.41422100
C	1.48203600	0.24795900	1.30974400
H	0.98530200	1.04677800	1.87269700
H	1.30577500	-0.68592900	1.86224100
C	3.07161200	-0.72573000	-0.99091900
H	3.26388500	0.18356100	-1.57724400
H	3.54681000	-1.54912400	-1.53925500
C	3.70296700	-0.58107500	0.40166200
C	2.99439500	0.50363700	1.22604300
H	3.18068400	1.48854600	0.77550600
H	3.41399700	0.54576000	2.23927500
H	4.77340300	-0.35629500	0.31343200
H	3.62731700	-1.54228000	0.93173500

Allene 6 B3LYP/6-31G*

0 1			
C	-0.70111300	-0.46556500	-0.05527500
C	-1.58525600	0.59343300	0.15267200
C	-1.14134000	1.90077600	0.56986100
C	0.73364700	-0.45071500	0.01947700
C	-0.00979300	2.32942700	-0.00108500
C	1.60352100	0.62031700	-0.16340000
C	1.13054800	1.93357300	-0.56785900
H	-1.67210300	2.45740100	1.34335900
H	1.64631000	2.49793100	-1.34526400

C	-3.00272500	0.08616300	0.03519500
H	-3.58393800	0.28146500	0.94993700
C	-2.82369500	-1.38415600	-0.23012400
H	-3.64494000	-2.07767100	-0.37237600
C	-1.51062700	-1.67989100	-0.27070000
H	-1.08746300	-2.66305600	-0.44911500
C	1.57463100	-1.69170600	0.25581000
H	1.33181200	-2.18679100	1.20790100
H	1.40871200	-2.44735300	-0.52728900
C	2.98334500	0.14759400	-0.01801800
H	3.85270000	0.79050100	-0.11013200
C	2.98847000	-1.17813200	0.22563900
H	3.85946200	-1.80814800	0.36781400
H	-3.54822100	0.58900600	-0.77798300

Allene 7 B3LYP/6-31G*

0 1

C	1.20292700	0.83211500	-0.09279600
C	1.49426700	2.19550100	-0.08359500
C	0.49284200	3.21868100	-0.33829900
C	-0.10353000	0.21917600	-0.18463800
C	-0.66871000	3.01607900	0.27823900
C	-1.33581500	0.76861600	0.18756800
C	-1.46306400	2.07047800	0.79119700
H	0.68490500	4.03815600	-1.03091200
H	-2.12458800	2.24218900	1.64079100
C	2.92818700	2.38850300	0.12186400
H	3.40129700	3.36357300	0.18094000
C	3.53497300	1.19347300	0.21849400
H	4.59727100	1.02970800	0.35712400
C	2.53770600	0.06612600	0.02531000
C	2.91444600	-0.68473500	-1.29566100
H	2.99086200	0.04646400	-2.10871500
H	2.11008000	-1.37320100	-1.57155600
C	2.54234600	-0.92643100	1.22247500
H	2.36112200	-0.36869400	2.14898400
H	1.70109500	-1.62230300	1.10811300
C	4.21630600	-1.49383100	-1.17042800
H	4.38802500	-2.04406800	-2.10459300
H	5.07186400	-0.81498300	-1.05330800
C	3.84605700	-1.73364500	1.32749800
H	3.76217500	-2.45235100	2.15282200
H	4.67915200	-1.06548100	1.58642100
C	4.16846500	-2.46647500	0.01707700
H	3.39671400	-3.22847300	-0.16971800
H	5.12086200	-3.00441400	0.10604200
C	-2.45994000	-0.23521300	-0.01952800
C	-0.38378800	-1.17699600	-0.58670900
H	0.36685600	-1.88624600	-0.90896700
C	-1.69939200	-1.44398000	-0.51063100

H	-2.16363600	-2.39058400	-0.76369400
C	-3.46662500	0.29871700	-1.08394100
H	-2.93922300	0.45133300	-2.03276500
C	-3.22427100	-0.52419400	1.30511500
H	-2.53019200	-0.94841200	2.04021200
C	-4.43421500	-1.45074200	1.10475500
H	-4.09099200	-2.44941900	0.80024700
H	-4.95361500	-1.58298900	2.06263600
C	-4.67802700	-0.62520000	-1.27915500
H	-5.36858000	-0.17143400	-2.00169100
H	-4.35177400	-1.57752300	-1.72061700
C	-5.40102100	-0.89822300	0.04764000
H	-5.84266200	0.03900400	0.41779000
H	-6.23382400	-1.59577600	-0.10789700
H	-3.81483900	1.28731400	-0.75436500
H	-3.57911200	0.43180600	1.71557700

Allene 8 B3LYP/6-31G*

0 1			
C	-0.79635600	-0.47408000	-0.31323000
C	-1.51942600	0.73176600	0.05515900
C	-1.00838100	1.95239400	-0.21463900
C	0.57462300	-0.54940200	-0.23401300
C	0.19007300	2.50835900	-0.43345500
C	1.51975800	0.51380500	0.13318900
C	1.37388300	1.87189400	0.11457400
H	0.31417100	3.39154100	-1.06374100
H	2.23000900	2.48233500	0.41071800
C	-2.82966900	0.30531400	0.55916400
H	-3.56291800	0.98498300	0.97968800
C	-3.00464500	-1.00850300	0.32050800
H	-3.90996300	-1.57294100	0.51836800
C	-1.78437000	-1.62667500	-0.33747800
H	-2.02146500	-1.98280900	-1.35336400
H	-1.40463100	-2.49788100	0.21254400
C	2.85013500	-0.15903400	0.46302800
H	3.69353100	0.29707600	-0.07405300
H	3.08498700	-0.06543600	1.53481200
C	1.35148700	-1.79374600	-0.30439600
H	0.92552500	-2.74311700	-0.61142400
C	2.62475100	-1.59550000	0.07846400
H	3.39958200	-2.35330900	0.12519900

Allene 9 B3LYP/6-31G*

0 1			
C	-1.18111500	0.77755200	-0.09991900
C	-1.34009100	2.14355600	0.37537800
C	-0.49932500	3.12722300	-0.01058100
C	0.06842600	0.25778900	-0.37837500

C	0.75213800	3.26271600	-0.45430300
C	1.38244800	0.90221400	-0.18294000
C	1.71437700	2.22501000	-0.12400100
H	1.05685900	4.07488600	-1.11767300
H	2.75893200	2.49322500	0.04005000
C	-2.61317000	2.21628500	1.09089500
H	-2.96055900	3.10219300	1.61198300
C	-3.30866100	1.08555800	0.88550300
H	-4.31912200	0.90690200	1.23578900
C	-2.52797300	0.04682800	0.07997300
C	0.36566700	-1.13546400	-0.74112000
H	-0.38276600	-1.84036400	-1.08058200
C	1.67409500	-1.40753900	-0.62128700
H	2.13131100	-2.36552600	-0.84269700
C	4.09664600	-1.45564800	1.40444600
H	4.45794100	-1.50755700	2.43955400
H	3.68112600	-2.44665100	1.17353000
C	5.26095800	-1.15234400	0.45023400
H	6.01524300	-1.94754800	0.50440400
H	5.75903000	-0.22603100	0.77334600
C	4.76916000	-0.98036400	-0.99439500
H	5.60418600	-0.69884900	-1.64859000
H	4.39762700	-1.94326300	-1.37205800
C	2.99037800	-0.39359500	1.30370600
H	2.15174900	-0.64520900	1.96349500
H	3.38649900	0.57153000	1.64971800
C	3.66554500	0.08565300	-1.09122300
H	4.10139600	1.05653900	-0.82293600
H	3.30664000	0.17801800	-2.12337000
C	2.46142000	-0.20372300	-0.15149800
C	-4.55655000	-0.97485600	-1.14664800
H	-5.28700000	-0.30901400	-0.66648100
H	-4.95701500	-1.20118500	-2.14315400
C	-3.78316700	-1.98561600	1.04731000
H	-3.63775900	-2.92533500	1.59551400
H	-4.47191400	-1.38210700	1.65396600
C	-3.20912200	-0.25050000	-1.28923200
H	-2.52944900	-0.87586000	-1.88537200
H	-3.33411300	0.68866700	-1.84095900
C	-2.42869600	-1.26769800	0.91083200
H	-2.01717300	-1.03498500	1.90015100
H	-1.72446300	-1.95790300	0.43650900
C	-4.41962800	-2.26357000	-0.32307500
H	-5.39894700	-2.74263700	-0.19742300
H	-3.79083200	-2.97873900	-0.87479600

Allene 10 B3LYP/6-31G*

0 1

C	0.619029	0.282144	-1.559582
C	-0.738015	-0.125259	-1.233634

C	-1.304362	-0.000202	-0.000005
C	1.677708	0.183678	-0.693531
C	-0.737944	0.125170	1.233587
C	1.677745	-0.183866	0.693614
C	0.619052	-0.282292	1.559649
H	2.669037	0.339282	-1.119138
H	2.669103	-0.339352	1.119189
C	-1.364906	-0.526214	-2.498755
H	-2.361709	-0.949787	-2.557996
C	-0.574046	-0.192644	-3.537520
H	-0.823865	-0.303061	-4.587632
C	0.719095	0.439891	-3.065755
H	1.613269	-0.057875	-3.464331
H	0.783732	1.492399	-3.387045
C	0.718964	-0.439745	3.065888
H	0.783462	-1.492201	3.387405
H	1.613219	0.057976	3.464339
C	-1.365043	0.526067	2.498587
H	-2.361934	0.949462	2.557654
C	-0.573989	0.193216	3.537461
H	-0.824052	0.303494	4.587530

Allene 11 B3LYP/6-31G*

0	1			
C		-0.044685	0.251319	-1.567359
C		-1.400453	-0.138274	-1.204159
C		-1.947265	-0.006489	0.035851
C		1.023849	0.169278	-0.716854
C		-1.364317	0.130202	1.262845
C		1.044587	-0.177366	0.702766
C		-0.007022	-0.261316	1.589886
C		-2.064533	-0.539922	-2.450382
H		-3.069610	-0.946788	-2.477828
C		-1.298397	-0.226333	-3.512228
H		-1.576419	-0.339933	-4.554871
C		0.021368	0.379024	-3.079673
H		0.886203	-0.156391	-3.494644
H		0.117777	1.421927	-3.423683
C		0.105890	-0.371047	3.100908
H		0.214022	-1.408621	3.457269
H		0.978875	0.175288	3.482698
C		-1.997716	0.538462	2.523106
H		-3.002706	0.943289	2.574159
C		-1.201849	0.234657	3.565817
H		-1.452189	0.352808	4.614884
C		2.456802	-0.320838	1.081021
H		2.778727	-0.610032	2.075536
C		3.268501	-0.044930	0.046403
H		4.352652	-0.076857	0.061353
C		2.469600	0.320674	-1.173884

H	2.707488	-0.325968	-2.031582
H	2.679024	1.348673	-1.507663

Allene 12 B3LYP/6-31G*

0	1		
C	1.59270100	0.02576300	-0.26375100
C	1.26812600	-1.32801700	0.11531700
C	0.04279400	-1.91282500	-0.00754700
C	0.68936500	1.08628600	-0.18197300
C	-1.19958900	-1.37349100	-0.12332300
C	-0.70891800	1.05693000	0.17806500
C	-1.56571300	-0.02622500	0.26158600
C	2.57209100	-2.01073300	0.51281100
H	2.68561300	-2.97598200	0.00563300
C	3.61802600	-1.00496100	0.10365300
H	4.68436200	-1.17428200	0.21437000
C	3.05204700	0.12792200	-0.36013400
C	-3.02807400	0.02417700	0.37797800
C	-2.48451600	-2.08983700	-0.52465400
H	-2.53824500	-2.28600000	-1.60860900
C	-3.55846000	-1.12295400	-0.09147900
H	-4.61970600	-1.32951400	-0.18892500
H	-2.56713600	-3.06727600	-0.03511300
H	2.62366800	-2.22649600	1.59319400
H	3.59264100	1.01095200	-0.68491100
H	-3.59193000	0.88451600	0.72406400
C	1.06667900	2.49807200	-0.32208600
H	2.06108800	2.82489700	-0.60545600
C	0.02763900	3.30658000	-0.04839300
H	0.03555700	4.39059000	-0.08104900
C	-1.18425500	2.49684000	0.31713800
H	-2.04176000	2.71780500	-0.33547300
H	-1.52380800	2.70963000	1.34303400

Allene 13 B3LYP/6-31G*

0	1		
C	0.50779600	2.32540700	0.51086000
C	1.27844000	1.27883100	0.93213500
C	1.21432100	-0.03267500	0.29874500
C	-0.50797500	2.32561400	-0.51012900
C	0.00025300	-0.55028900	-0.00085400
C	-1.27839400	1.27918000	-0.93210000
C	-1.21416300	-0.03248400	-0.29880900
H	0.71395400	3.29693200	0.95902400
H	2.02130900	1.46956000	1.70835400
H	-0.71397800	3.29731000	-0.95800400
H	-2.02080200	1.46989000	-1.70875800
N	2.40933300	-0.74848000	0.13191600

N	-2.40888400	-0.74798400	-0.13054200
C	3.65224600	-0.04361700	-0.14370600
H	4.50076400	-0.63419300	0.22190100
H	3.80128800	0.13055200	-1.22397100
H	3.67039200	0.92457300	0.35707900
C	2.32448300	-2.04864200	-0.50874700
H	3.23586500	-2.61654400	-0.28839400
H	1.45169700	-2.57822600	-0.11954500
H	2.21639900	-1.98006100	-1.60426200
C	-3.65280500	-0.04414300	0.14262500
H	-3.66854500	0.92615500	-0.35411000
H	-4.50020700	-0.63292500	-0.22855100
H	-3.80594100	0.12563300	1.22299600
C	-2.32441900	-2.04859800	0.50903200
H	-3.23465000	-2.61734000	0.28588900
H	-1.45004500	-2.57679500	0.12153000
H	-2.21934000	-1.98077400	1.60488400

Allene 14 B3LYP/6-31G*

0	1		
C	0.33338100	1.63392900	-0.32222900
C	1.40704500	0.74488300	-0.38753700
C	1.37896600	-0.57511000	0.20686700
C	-0.95728700	1.41335000	0.25715800
C	0.22619300	-1.28644700	0.15744800
C	-1.61538000	0.21159400	0.46986500
C	-1.08822900	-1.04903400	-0.03564400
C	2.60990500	1.48991400	-0.92719700
H	3.43405600	1.47402000	-0.19887700
C	2.09149300	2.88019500	-1.17003300
H	2.68940600	3.68467100	-1.58353800
C	0.79708500	2.94501800	-0.81081400
H	0.16190400	3.82280500	-0.87289300
C	-1.84698000	2.52880400	0.77651700
H	-1.33732800	3.14708300	1.53010900
H	-2.14367100	3.21917300	-0.02813500
C	-2.88474000	0.47529100	1.15948900
H	-3.57470500	-0.30384500	1.46573900
C	-3.03502800	1.80159100	1.34597100
H	-3.87049100	2.29817100	1.82669900
H	3.00520100	1.03542500	-1.84813500
N	2.55605700	-1.03859800	0.88515200
N	-1.95524800	-1.98275600	-0.62102700
C	3.58624000	-1.55760800	-0.01612300
H	4.50000100	-1.76180400	0.55371700
H	3.26979800	-2.49136400	-0.51657100
H	3.82814400	-0.82639900	-0.79040300
C	2.25677300	-2.00400100	1.93543800
H	1.80543500	-2.93321100	1.54520600
H	3.18475300	-2.25392900	2.46137000

H	1.55623600	-1.56480400	2.65103800
C	-1.36377600	-3.22408800	-1.09327600
H	-0.63909800	-3.57394100	-0.35391600
H	-2.15659800	-3.96936000	-1.22500000
H	-0.83539700	-3.10803800	-2.05421600
C	-3.06190200	-1.51797600	-1.44751800
H	-2.74770200	-1.31689800	-2.48632700
H	-3.84325000	-2.28638800	-1.47418100
H	-3.49491500	-0.60370500	-1.04084900

Allene 15 B3LYP/6-31G*

0 1			
C	1.60457400	0.11550700	-0.28243100
C	1.19674500	-1.24947600	0.06619100
C	-0.02163500	-1.83587400	-0.18395500
C	0.72140400	1.19222300	-0.31743800
C	-1.24210700	-1.23313100	-0.38317000
C	-0.70889800	1.20559200	-0.07601700
C	-1.60078000	0.12816500	0.01597700
C	2.36765400	-1.92788900	0.55374900
H	2.34129000	-2.95066500	0.90726300
C	3.48672600	-1.14930700	0.37641700
C	3.07413000	0.13884900	-0.24298100
C	-3.05956600	0.16500400	0.12505400
C	-2.45744600	-1.87711800	-0.80938800
C	-3.54567300	-1.08944800	-0.50984500
C	-1.12537800	2.61772300	-0.07249900
H	-2.15171800	2.93890100	0.03393500
C	-0.08497500	3.43765900	-0.28462700
H	-0.12531000	4.51928300	-0.35357600
C	1.16748900	2.64042400	-0.48041600
H	1.96254800	2.91106800	0.22864500
H	1.57784900	2.82624700	-1.48468600
C	3.89174000	1.13111900	-0.73172700
H	3.40335400	1.95382900	-1.24164900
C	5.30636500	1.23582400	-0.69746100
C	6.25583500	0.36695900	-0.16424900
C	4.83344000	-1.54208000	0.71178600
C	6.03423200	-0.88477800	0.48239600
H	-2.48054500	-2.89004500	-1.19101200
C	-4.92370800	-1.44390800	-0.73639000
C	-6.08437200	-0.79668500	-0.33188600
C	-3.80127000	1.10647200	0.80246200
H	-3.23736800	1.86868200	1.33367500
C	-5.20695700	1.21070700	0.94560900
C	-6.21883800	0.39210200	0.44331600
C	-5.31236500	-2.64169300	-1.49333600
H	-4.60091600	-3.32748400	-1.93758000
C	-6.65366600	-2.73983700	-1.55882600
H	-7.22016300	-3.51743000	-2.05873100

C	-7.50816700	0.95528100	0.86347900
H	-8.46831300	0.51921300	0.60930300
C	-7.31813800	2.06783900	1.60031400
H	-8.09005400	2.68646100	2.04382600
C	5.13297500	-2.80268000	1.40586300
H	4.37588800	-3.51225300	1.71711900
C	6.45956100	-2.92775700	1.59913000
H	6.96560700	-3.75264200	2.08794400
C	7.58393100	0.95421500	-0.38213400
H	8.50980900	0.48680300	-0.06437400
C	7.47657000	2.13340500	-1.02612900
H	8.29237000	2.78410000	-1.31985300
C	7.16432400	-1.73152700	1.03264200
H	7.88568600	-2.01523400	0.25064300
H	7.74670400	-1.19755100	1.79948700
C	6.02977800	2.42850100	-1.29099900
H	5.71178700	3.37504100	-0.82672000
H	5.82357900	2.53852700	-2.36722100
C	-5.84844100	2.33891700	1.72879800
H	-5.52180600	2.34367500	2.78050600
H	-5.57596700	3.32705200	1.32645800
C	-7.27797600	-1.58838300	-0.82842600
H	-7.91873600	-1.93071600	-0.00108600
H	-7.92830300	-0.99034500	-1.48544500

Allene 16 B3LYP/6-31G*

0 1			
C	-1.60631000	0.31630400	0.30764800
C	-1.26496600	-1.08565200	-0.09811900
C	0.01206400	-1.45818900	-0.01736100
C	-0.68421000	1.38739200	0.17737400
C	1.28262200	-1.06051500	0.07473800
C	0.67918100	1.40456500	-0.20194100
C	1.62273600	0.33479200	-0.31478200
C	-2.48266700	-1.80816200	-0.42369700
H	-2.51764500	-2.85038800	-0.71435100
C	-3.51808700	-0.96876500	-0.08376400
C	-3.01150200	0.33596700	0.33486900
C	3.02922600	0.36026200	-0.32623900
C	2.50037700	-1.79409400	0.39430200
H	2.53031300	-2.83983900	0.67346600
C	3.53661500	-0.95513400	0.06924700
C	1.07251000	2.81222900	-0.36577800
H	2.06471300	3.11894900	-0.67447600
C	0.05013900	3.63778600	-0.08199300
H	0.06634200	4.72130800	-0.11208700
C	-1.15458900	2.82714700	0.29820200
H	-2.01296900	3.02840300	-0.35951400
H	-1.49644800	3.05213000	1.32023200
C	-4.12676100	1.19985000	0.50415600

H	-4.09895200	2.24059200	0.80503300
C	4.14877900	1.22383500	-0.45740200
H	4.13340400	2.27371800	-0.72460200
C	5.32385200	0.50524900	-0.23504400
C	4.98818200	-0.90655100	0.09073900
C	-4.97028700	-0.91605900	-0.09360000
C	-5.30393100	0.48910000	0.27517900
C	5.82634400	-1.95108000	0.36310800
H	5.34802100	-2.90712100	0.56958600
C	6.63757500	1.05302900	-0.31908400
H	6.67223400	2.11341600	-0.56721300
C	-5.81107100	-1.95091200	-0.38940500
H	-5.33524600	-2.90100200	-0.62734300
C	-6.61692200	1.03181100	0.39051900
H	-6.64929400	2.08374200	0.67326900
C	7.25747500	-1.96010800	0.41550900
H	7.70158900	-2.92365800	0.65667300
C	8.12991700	-0.92617000	0.20389500
H	9.18733900	-1.16581700	0.29817000
C	7.84814400	0.43901500	-0.12828600
H	8.72480700	1.07287700	-0.24375500
C	-7.24383100	-1.95818000	-0.43163900
H	-7.69025600	-2.91343800	-0.69991000
C	-8.11292000	-0.93097600	-0.18043900
H	-9.17128000	-1.16752200	-0.27380500
C	-7.82953000	0.42405100	0.19292000
H	-8.70559100	1.05262600	0.33764300

Allene 17 B3LYP/6-31G*

0 1			
C	1.60225200	-0.78999300	0.33125100
C	1.26485800	0.60611200	-0.07178600
C	-0.00953700	1.00203900	-0.00738600
C	0.68354000	-1.86154400	0.18737200
C	-1.27775800	0.58232500	0.06595000
C	-0.67423100	-1.87690100	-0.21212900
C	-1.61357900	-0.80532400	-0.33695400
C	2.49083200	1.33187900	-0.37478800
H	2.51935100	2.37494600	-0.65837600
C	3.52598700	0.49566700	-0.02465100
C	3.00829500	-0.81124100	0.38649700
C	-3.02078000	-0.83112000	-0.38122100
C	-2.50347500	1.31331400	0.37131000
H	-2.52788800	2.35667200	0.65478200
C	-3.53908000	0.48052300	0.02510400
C	-1.06671900	-3.28451100	-0.37950400
H	-2.05579200	-3.59034000	-0.69906100
C	-0.04905300	-4.11133600	-0.08223700
H	-0.06616100	-5.19494100	-0.11261700
C	1.15101300	-3.30161000	0.31483100

H	2.01956600	-3.50306100	-0.32958900
H	1.47783300	-3.52674600	1.34185600
C	4.11340400	-1.67279000	0.58289900
H	4.07931800	-2.71219000	0.88793700
C	-4.13106300	-1.68857200	-0.56298900
H	-4.10940200	-2.73149800	-0.85613100
C	-5.31634400	-0.97379300	-0.35659600
C	-4.99402800	0.42609400	0.01300700
C	4.98090100	0.43646500	-0.00802400
C	5.30074100	-0.96277200	0.37594800
C	-5.85127200	1.45312000	0.29818800
C	-6.61710400	-1.53381100	-0.49542400
H	-6.62862700	-2.58930700	-0.77029600
C	5.84037800	1.45884300	-0.30106700
C	6.60054000	-1.52148300	0.52643100
H	6.61001200	-2.57373900	0.81402800
C	-7.30480200	1.46806900	0.30104200
C	-8.17064500	0.42450000	0.02682700
C	-7.83938200	-0.94178000	-0.33197400
C	7.29477100	1.47091000	-0.30282900
C	8.15738900	0.42893900	-0.01464300
C	7.82416800	-0.93317700	0.36027900
C	-9.63103400	0.51591800	0.05498700
H	-10.17368700	1.42351500	0.29355900
C	-10.19607600	-0.66735000	-0.25052200
H	-11.26097600	-0.86781200	-0.29836400
C	7.70908800	2.82400300	-0.67273200
H	8.74411500	3.13618500	-0.75273500
C	6.64155700	3.61336300	-0.89515700
H	6.67338100	4.65841900	-1.18354400
C	9.61795500	0.51820100	-0.04081700
H	10.16221500	1.42214700	-0.28948400
C	10.18104900	-0.66170700	0.28097100
H	11.24575200	-0.86223900	0.33397500
C	-9.14406900	-1.70514800	-0.52316200
H	-9.22914100	-2.12395500	-1.53763100
H	-9.22222800	-2.56215200	0.16339200
C	9.12770100	-1.69520900	0.56477100
H	9.20780200	-2.56147100	-0.10993500
H	9.21104900	-2.10040700	1.58504000
C	5.36330500	2.84711100	-0.69668100
H	4.71850600	3.29108900	0.07781500
H	4.75107100	2.81688700	-1.61133600
C	-5.37105500	2.84419400	0.67916800
H	-4.76080500	2.82300000	1.59532100
H	-4.72432500	3.27842700	-0.09913100
C	-7.71672600	2.82618600	0.65535900
H	-8.75110900	3.14116700	0.73192900
C	-6.64741300	3.61563000	0.86838800
H	-6.67681100	4.66398800	1.14476100

Allene 18 B3LYP/6-31G*

0	1			
C		-1.59602800	-0.94569900	-0.38925900
C		-1.26398800	0.43879500	0.05785400
C		0.00853500	0.85303700	0.02009400
C		-0.68009000	-2.01652000	-0.26434800
C		1.27308900	0.40767100	-0.04956600
C		0.67233600	-2.05449800	0.15814700
C		1.60516900	-0.98424100	0.31780800
C		-2.49866000	1.14919000	0.36807600
H		-2.53230500	2.18418700	0.68021300
C		-3.52820800	0.32338800	-0.02471800
C		-3.00341500	-0.96688300	-0.47623700
C		3.01609600	-1.01634000	0.37878400
C		2.50658800	1.14421900	-0.32179000
H		2.53149300	2.19503700	-0.57854000
C		3.54058600	0.30523800	0.01153900
C		1.05821900	-3.45530700	0.32633200
H		2.03579400	-3.76133900	0.67129900
C		0.03329800	-4.28439100	-0.00947400
C		-1.16012500	-3.44954700	-0.41341200
H		-2.03786500	-3.63643900	0.22134300
H		-1.47104500	-3.66972300	-1.44533600
C		-4.10507000	-1.81697700	-0.72934900
H		-4.06652700	-2.84293200	-1.07851300
C		4.12025600	-1.87689600	0.54976700
H		4.09490100	-2.92755100	0.81467000
C		5.31422000	-1.15747800	0.37115800
C		4.99707900	0.24634500	0.03610900
C		-4.98455100	0.26253000	-0.06836300
C		-5.29906900	-1.11494000	-0.51534000
C		5.86122500	1.27744200	-0.21555500
C		6.61252700	-1.71593500	0.50535100
H		6.62822900	-2.77792900	0.75509800
C		-5.85009400	1.27051400	0.25564200
C		-6.59864300	-1.65655300	-0.71291200
H		-6.61185400	-2.69576100	-1.04622700
C		7.31048800	1.30900600	-0.21521400
C		8.18081600	0.25390300	0.04121700
C		7.83408800	-1.11251200	0.36219100
C		-7.30162900	1.30406700	0.23957300
C		-8.16715300	0.27604300	-0.11106500
C		-7.81980600	-1.06367700	-0.54339800
C		9.63033400	0.35164600	0.03405700
H		10.16681000	1.26986600	-0.16388000
C		10.20647200	-0.85571400	0.30754700
C		-7.71238200	2.63441500	0.65273600
H		-8.74570000	2.94876800	0.71503300
C		-6.63093500	3.41592700	0.94245400
C		-9.61663900	0.36890400	-0.09409000

H	-10.15478500	1.25801300	0.20616300
C	-10.19125500	-0.80144100	-0.49898500
C	9.12981600	-1.88850600	0.55464700
H	9.19034800	-2.31714900	1.56560400
H	9.21122200	-2.73276600	-0.14590800
C	-9.11576000	-1.82000000	-0.80391300
H	-9.19643400	-2.71038600	-0.16282900
H	-9.18256400	-2.17899700	-1.84193000
C	-5.35876700	2.63237700	0.71228400
H	-4.70539300	3.09027900	-0.04546800
H	-4.75406100	2.55655000	1.62861000
C	5.36709500	2.66830400	-0.57042800
H	4.76689200	2.64776600	-1.49196000
H	4.71113800	3.07820400	0.21212900
C	7.72127500	2.66155100	-0.54218100
H	8.75482500	2.97014800	-0.62344800
C	6.63732900	3.47149200	-0.73279400
N	0.03088800	-5.66754000	-0.07898000
C	1.20828500	-6.35122800	0.42361100
H	2.10212500	-5.94407700	-0.05975600
H	1.33118700	-6.24725800	1.51570600
H	1.14068400	-7.41586300	0.18030800
C	-1.22750900	-6.37574500	0.09832100
H	-1.57068300	-6.39629200	1.14774300
H	-2.00986900	-5.91199200	-0.50702700
H	-1.10858700	-7.40964300	-0.24190100
N	-11.53022500	-1.06785800	-0.69172800
N	-6.61959300	4.69992700	1.44413300
N	6.62293500	4.82537500	-0.97700100
N	11.54628000	-1.17694900	0.30736200
C	7.89733700	5.48583600	-1.19774700
H	7.74652400	6.56895800	-1.20472700
H	8.58562100	5.24029100	-0.38286900
H	8.36933100	5.19092000	-2.14969400
C	5.46875100	5.43702600	-1.61953300
H	4.54452500	5.01878300	-1.21625400
H	5.46971300	6.51197600	-1.41280000
H	5.46360500	5.29747500	-2.71368100
C	-12.48278900	-0.04781400	-0.29025000
H	-12.20618700	0.91142600	-0.73889600
H	-13.47830500	-0.32095400	-0.65161600
H	-12.53038000	0.08391200	0.80381100
C	-12.00960400	-2.44042900	-0.62609100
H	-12.98674700	-2.50328200	-1.11559900
H	-11.32599500	-3.10655800	-1.15643300
H	-12.11971900	-2.80935300	0.40809700
C	-5.45905600	5.55065900	1.22597400
H	-5.47150300	6.36919900	1.95286700
H	-4.53894500	4.98253800	1.37671700
H	-5.43216400	5.99030800	0.21424000
C	-7.89287100	5.38720700	1.56235500
H	-8.60148200	4.75751300	2.10971900

H	-7.75206100	6.31438700	2.12523700
H	-8.33661500	5.63507100	0.58329100
C	12.49750700	-0.09272200	0.13600500
H	12.23550000	0.48984900	-0.75277500
H	12.52468500	0.59063200	1.00119000
H	13.49783200	-0.50983500	-0.00999500
C	12.01639500	-2.31504500	1.08358100
H	12.10541400	-2.09354200	2.16077600
H	11.33892400	-3.16282600	0.96257600
H	13.00175100	-2.61844300	0.71589200

Allene 19 B3LYP/6-31G*

0 1			
C	-1.59802500	0.88622300	0.63319500
C	-1.23202400	-0.49751100	0.24903800
C	0.03391700	-0.96228800	0.29601500
C	-0.74949100	1.95807200	0.48718200
C	1.26968900	-0.41739900	0.34658200
C	0.65055900	2.00198100	0.06713200
C	1.56656700	0.96993100	-0.06896500
C	-2.46211100	-1.21309000	-0.07113400
H	-2.46635000	-2.23416900	-0.43360000
C	-3.53529400	-0.42698300	0.26188800
C	-3.04477900	0.88391800	0.72887100
C	3.01133400	1.03334000	-0.17602900
C	2.53236200	-1.07091100	0.67628300
H	2.58415100	-2.08536500	1.05288600
C	3.56482600	-0.24492300	0.31668300
C	0.99132300	3.41820100	-0.09948800
H	1.96895500	3.75659200	-0.42036200
C	-0.04933000	4.21228200	0.20701300
H	-0.05451100	5.29636100	0.17132100
C	-1.23573500	3.39144400	0.62707400
H	-2.12524600	3.57941000	0.00617100
H	-1.53992500	3.61310000	1.66171700
C	-4.13227000	1.67085200	0.98582400
H	-4.14976200	2.69061500	1.35322000
C	4.06560500	1.85387900	-0.46856100
H	4.04352300	2.86527400	-0.85827600
C	5.30765700	1.12904300	-0.21092100
C	5.00782600	-0.16829700	0.27136800
C	-4.98129500	-0.40147900	0.27089300
C	-5.34083800	0.89291700	0.71692400
C	5.93956000	-1.15039700	0.72729300
C	6.58520200	1.71650700	-0.43801100
H	6.56770000	2.75563900	-0.76497600
C	-5.86564600	-1.48750200	-0.01543200
C	-6.64504500	1.43367800	0.91136900
H	-6.67249500	2.44649600	1.31201000
C	7.32465800	-1.17840800	0.63083900

C	8.20511700	-0.23001600	-0.04854600
C	7.81998300	1.12400900	-0.37325700
C	-7.25012100	-1.50816400	-0.11313800
C	-8.18226700	-0.38428000	-0.03559100
C	-7.85515100	0.88186400	0.58036100
C	9.54623300	-0.43698300	-0.41745200
C	10.15796000	0.81699000	-0.82066500
C	-7.66951100	-2.91196400	-0.25177700
H	-8.70305700	-3.23391900	-0.27332400
C	-6.59868000	-3.72827300	-0.29949300
H	-6.60989700	-4.80772900	-0.39409400
C	-9.52156300	-0.36731400	-0.46077100
C	-10.18930400	0.82920300	0.02196100
C	9.07428300	1.87250200	-0.77262900
H	8.95861500	2.38327500	-1.73696200
H	9.31770000	2.65157300	-0.03591800
C	-9.14575500	1.65783500	0.74044700
H	-9.07139900	2.67089400	0.32535800
H	-9.40278600	1.77573900	1.80301400
C	-5.35238700	-2.90474400	-0.17955200
H	-4.73109100	-3.21099400	0.67430900
H	-4.71138200	-2.99677200	-1.06980900
C	5.48924600	-2.36670100	1.51255400
H	4.88038300	-2.08351900	2.38313900
H	4.85424700	-3.02369400	0.89841900
C	7.80497700	-2.33467600	1.40434700
H	8.85156200	-2.55994700	1.56676700
C	6.77080500	-3.03378100	1.91131000
H	6.82931900	-3.92546100	2.52432000
C	10.20277900	-1.72551200	-0.52905500
H	9.54581900	-2.58440800	-0.42939900
C	-10.13205700	-1.31753100	-1.37143900
H	-9.44186500	-2.01447300	-1.83764200
C	-11.42726300	-1.42485300	-1.77088800
H	-11.63453100	-2.21649500	-2.48901200
C	-12.58155500	-0.63437500	-1.39559700
H	-13.53437200	-0.99240400	-1.77994000
C	11.50401600	-2.01403700	-0.79845600
H	11.74982900	-3.07320900	-0.85360800
C	12.62042100	-1.12295500	-1.03748100
H	13.59025100	-1.60765100	-1.12823900
C	11.44633000	1.10984600	-1.15396600
H	11.65884200	2.15132500	-1.39075500
C	12.58641700	0.22550500	-1.20191400
H	13.53639300	0.71553100	-1.40926600
C	-11.49441700	1.21142300	-0.05839900
H	-11.75102500	2.15552100	0.41993600
C	-12.60172200	0.51108800	-0.66516100
H	-13.57370500	0.97973600	-0.51946500

PROTONATED B3LYP

Allene 1H B3LYP/6-31G*

1	1			
C		0.697708	0.000000	1.453263
C		-0.701008	0.000000	1.451673
C		-1.571936	0.000000	0.356899
C		1.571120	0.000000	0.360470
C		-1.259264	0.000000	-1.006646
C		1.261548	0.000000	-1.003781
C		0.001831	0.000000	-1.611925
H		1.168796	0.000000	2.433381
H		-1.174322	0.000000	2.430718
H		-2.632332	0.000000	0.598007
H		2.630966	0.000000	0.603987
H		-2.108705	0.000000	-1.685585
H		2.112529	0.000000	-1.680788
H		0.003067	0.000000	-2.699429

Allene 2H B3LYP/6-31G*

1	1			
C		0.50468300	-0.69603500	0.00012600
C		0.49711500	0.73423000	0.00011100
C		-0.61809000	1.59249200	0.00019900
C		-0.56619400	-1.57415900	0.00011500
C		-1.96431300	1.25071500	0.00000900
C		-1.93991100	-1.27214000	-0.00008600
C		-2.55641600	-0.02566200	-0.00019200
H		-0.39535400	2.65718300	0.00036400
H		-0.31776700	-2.63377400	0.00019100
H		-2.65977800	2.08654000	0.00003900
H		-2.60674700	-2.13075700	-0.00022900
H		-3.64347000	-0.03609300	-0.00040200
C		1.87198000	1.19715100	-0.00011900
H		2.15456000	2.24349100	-0.00007000
C		2.71269600	0.13617700	-0.00023300
H		3.79573200	0.18313600	-0.00059500
C		1.94562200	-1.14715500	0.00013500
H		2.17496600	-1.77159800	0.87709400
H		2.17482200	-1.77181900	-0.87679200

Allene 3H B3LYP/6-31G*

1	1			
C		0.66956400	-0.14292100	-0.00008900
C		1.41022100	1.08243800	-0.00007800
C		2.80541600	1.26018900	0.00005300
C		1.16487400	-1.43691500	0.00006600
C		2.50290200	-1.86949600	0.00019900

C	3.66736300	-1.10945900	0.00015300
H	3.14743100	2.29291000	0.00010600
H	0.42378300	-2.23299100	0.00009300
H	2.64291900	-2.94772300	0.00033900
H	4.59921700	-1.66924500	0.00022300
C	0.46409800	2.17785600	-0.00046600
H	0.75154100	3.22309600	-0.00042200
C	-0.79561300	1.68661200	-0.00074200
H	-1.69557500	2.29008000	-0.00112800
C	-0.81737800	0.18191400	-0.00022500
C	-1.53137600	-0.38495900	1.27733900
H	-1.06548000	0.03867900	2.17413000
H	-1.36084600	-1.46866200	1.30838900
C	-1.53159300	-0.38615600	-1.27711600
H	-1.06582800	0.03664800	-2.17435500
H	-1.36110800	-1.46988400	-1.30712500
C	-3.04431400	-0.11847500	1.26826600
H	-3.48163700	-0.58043300	2.16072000
H	-3.23675900	0.95908400	1.35811900
C	-3.04453200	-0.11962400	-1.26807100
H	-3.48199200	-0.58239500	-2.16004000
H	-3.23699800	0.95785000	-1.35889900
C	-3.71387500	-0.66592000	0.00040300
H	-3.65019200	-1.76344200	0.00090200
H	-4.78037400	-0.41660900	0.00038400
C	3.79946300	0.28984400	0.00005600
H	4.82058100	0.66346800	0.00006400

Allene 4H B3LYP/6-31G*

1 1			
C	-0.50472300	-0.69616100	-0.00000200
C	-0.49711500	0.73419800	-0.00000300
C	0.61809900	1.59248100	0.00000000
C	0.56629600	-1.57417000	-0.00000200
C	1.96427600	1.25078800	0.00000100
C	1.93995600	-1.27215600	-0.00000100
C	2.55641000	-0.02563000	0.00000000
H	2.65983900	2.08651500	0.00000000
H	3.64345400	-0.03590400	-0.00000100
C	-1.87198600	1.19717700	0.00000600
H	-2.15466000	2.24348500	0.00001500
C	-2.71270200	0.13619000	-0.00001200
H	-3.79573900	0.18303900	-0.00001400
C	-1.94564500	-1.14711300	0.00000800
H	-2.17498200	-1.77173000	-0.87689600
H	-2.17497900	-1.77171000	0.87692900
H	0.39519000	2.65713800	0.00000200
H	0.31780400	-2.63377200	0.00000000
H	2.60687300	-2.13068000	-0.00000200

Allene 5H B3LYP/6-31G*

1	1			
C		-0.66956700	-0.14293400	-0.00028600
C		-1.41022200	1.08243600	-0.00006200
C		-2.80540000	1.26019100	0.00017700
C		-1.16489800	-1.43690900	-0.00007600
C		-3.79947000	0.28987200	0.00020600
C		-2.50293400	-1.86948000	0.00027900
C		-3.66739300	-1.10943600	0.00027000
H		-0.42380600	-2.23298600	0.00020200
H		-4.82058200	0.66350500	0.00020800
H		-2.64295600	-2.94770700	-0.00016600
H		-4.59926600	-1.66919000	0.00017100
C		-0.46409000	2.17783200	-0.00072800
H		-0.75151500	3.22307400	-0.00084900
C		0.79561100	1.68656600	-0.00104500
H		1.69558900	2.29001500	-0.00156100
C		0.81738700	0.18188000	-0.00042000
C		1.53174400	-0.38632600	-1.27711300
H		1.06608300	0.03635300	-2.17447100
H		1.36125100	-1.47006100	-1.30704100
C		1.53124700	-0.38480100	1.27734300
H		1.06520900	0.03896700	2.17399700
H		1.36071900	-1.46850200	1.30851900
C		3.04467700	-0.11983700	-1.26794200
H		3.23716700	0.95761900	-1.35898300
H		3.48223000	-0.58277100	-2.15978500
C		3.71390800	-0.66585400	0.00069700
C		3.04416600	-0.11829100	1.26840700
H		3.23658500	0.95928300	1.35817900
H		3.48137300	-0.58012500	2.16098700
H		4.78038900	-0.41645100	0.00075800
H		3.65036000	-1.76338800	0.00135000
H		-3.14741800	2.29291300	0.00023900

Allene 6H B3LYP/6-31G*

1	1			
C		0.67811200	-0.57383900	0.00005000
C		1.56982300	0.55112500	0.00000800
C		1.27829000	1.90080100	-0.00007800
C		-0.71770500	-0.54832200	0.00010800
C		0.01437300	2.52742700	-0.00005700
C		-1.58087000	0.58027700	0.00004100
C		-1.24380400	1.95127900	-0.00006100
H		2.13272300	2.57467200	0.00032100
H		-2.08509900	2.64051900	-0.00006400
C		2.98598300	0.01908300	-0.00000600
H		3.55065300	0.36850200	0.87735600
C		2.79964300	-1.46528300	-0.00006500

H	3.62388400	-2.16940700	0.00000800
C	1.48742400	-1.78557700	-0.00001000
H	1.07962500	-2.78887700	-0.00008400
C	-1.58006600	-1.78954000	0.00004500
H	-1.38392100	-2.42319800	-0.87801700
H	-1.38400400	-2.42358600	0.87778700
C	-2.95674700	0.10395500	0.00009300
H	-3.81821100	0.76173900	0.00023600
C	-2.97504100	-1.24633200	-0.00012600
H	-3.85865300	-1.87395200	-0.00020200
H	0.03573500	3.61433000	0.00007100
H	3.55079300	0.36894800	-0.87705600

Allene 7H B3LYP/6-31G*

1 1

C	1.19969600	0.77475600	-0.00005200
C	1.47056200	2.17577900	0.00028000
C	0.58547700	3.27351700	0.00000800
C	-0.06504900	0.16603800	-0.00033400
C	-0.79569000	3.26610600	-0.00022400
C	-1.35546600	0.81147000	-0.00031000
C	-1.66247100	2.15794500	-0.00022900
H	1.06003400	4.25221500	0.00004500
H	-2.72136400	2.40483600	-0.00023300
C	2.90831200	2.36910200	0.00075900
H	3.38071100	3.34495900	0.00129400
C	3.52640300	1.17292900	0.00043300
H	4.59916000	1.02400500	0.00060600
C	2.54415400	0.03139700	0.00007500
C	2.74939600	-0.83681100	-1.29115500
H	2.70571800	-0.18271100	-2.16959000
H	1.91921200	-1.54336300	-1.38821300
C	2.74900000	-0.83733800	1.29099800
H	2.70498000	-0.18364400	2.16971100
H	1.91885100	-1.54401200	1.38746900
C	4.06935500	-1.62433300	-1.26737900
H	4.11191200	-2.25645100	-2.16187200
H	4.92204900	-0.93634700	-1.34071900
C	4.06901200	-1.62476900	1.26730400
H	4.11146400	-2.25713000	2.16162800
H	4.92163800	-0.93672400	1.34106400
C	4.20330100	-2.47995900	-0.00017200
H	3.42503000	-3.25723200	-0.00042300
H	5.16497700	-3.00466400	-0.00014300
C	-2.45350100	-0.24940100	-0.00038300
C	-0.31962800	-1.27187100	-0.00062600
H	0.44474400	-2.03367800	-0.00070700
C	-1.64541600	-1.51427800	-0.00075500
H	-2.08992100	-2.50244600	-0.00111500
C	-3.35696700	-0.14480000	-1.27548100

H	-2.73717200	-0.26058500	-2.17200100
C	-3.35597800	-0.14526700	1.27561500
H	-2.73540400	-0.26140900	2.17154300
C	-4.50243800	-1.16842200	1.26909200
H	-4.09825600	-2.18597400	1.35802400
H	-5.11847000	-1.00731700	2.16121200
C	-4.50342200	-1.16797000	-1.26844400
H	-5.12013900	-1.00655600	-2.16003200
H	-4.09931300	-2.18549200	-1.35804200
C	-5.35980000	-1.05612600	0.00067500
H	-5.88203200	-0.08862900	0.00105200
H	-6.13635500	-1.82878600	0.00084600
H	-3.78390300	0.86556100	-1.31149800
H	-3.78281300	0.86511200	1.31230600
H	-1.27837500	4.24030900	-0.00037900

Allene 8H B3LYP/6-31G*

1 1			
C	-0.71772300	-0.54829900	-0.00001300
C	-1.58086500	0.58027000	0.00000900
C	-1.24382200	1.95126700	0.00000100
C	0.67811400	-0.57379900	-0.00000800
C	0.01438700	2.52739400	0.00002500
C	1.56982700	0.55112000	0.00001900
C	1.27828600	1.90077000	-0.00002200
H	0.03572200	3.61430800	-0.00029200
H	2.13276400	2.57460100	-0.00005700
C	-2.95673800	0.10394600	0.00007100
H	-3.81820000	0.76173800	0.00009700
C	-2.97501900	-1.24632600	-0.00006600
H	-3.85865300	-1.87392400	-0.00012300
C	-1.58005200	-1.78954900	0.00001800
H	-1.38389700	-2.42338600	-0.87788100
H	-1.38394500	-2.42331500	0.87798900
C	2.98599200	0.01905000	0.00006700
H	3.55074000	0.36879900	-0.87712300
H	3.55067400	0.36872400	0.87731300
C	1.48740300	-1.78554400	0.00001300
H	1.07964700	-2.78885900	0.00001600
C	2.79961600	-1.46525900	-0.00008100
H	3.62380400	-2.16946400	-0.00006200
H	-2.08509100	2.64054100	-0.00008000

Allene 9H B3LYP/6-31G*

1 1			
C	1.19973200	0.77480400	-0.00004600
C	1.47060600	2.17581900	0.00006600
C	-0.06500300	0.16608500	-0.00015400
C	-0.79564700	3.26612800	0.00006400

C	-1.35542800	0.81150700	-0.00017300
C	-1.66242600	2.15798400	-0.00000900
H	-1.27834100	4.24032600	0.00015100
H	-2.72131500	2.40488500	0.00015800
C	2.90835600	2.36912900	0.00017500
H	3.38076100	3.34498400	0.00018100
C	3.52643000	1.17294400	0.00015400
H	4.59918700	1.02401900	0.00014300
C	2.54416800	0.03140700	0.00001600
C	-0.31954800	-1.27183000	-0.00027900
H	0.44485800	-2.03361400	-0.00023600
C	-1.64533200	-1.51424800	-0.00033700
H	-2.08983100	-2.50242000	-0.00044700
C	-4.50309600	-1.16803700	-1.26867700
H	-5.11961600	-1.00662500	-2.16039600
H	-4.09895900	-2.18555500	-1.35814100
C	-5.35974100	-1.05610600	0.00025500
H	-6.13628300	-1.82877500	0.00030500
H	-5.88196200	-0.08860900	0.00046500
C	-4.50264400	-1.16834700	1.26886700
H	-5.11888400	-1.00717600	2.16082900
H	-4.09850300	-2.18589800	1.35794100
C	-3.35662000	-0.14486500	-1.27552400
H	-2.73662000	-0.26075900	-2.17188600
H	-3.78352400	0.86550000	-1.31171500
C	-3.35618100	-0.14519500	1.27558600
H	-3.78304000	0.86517100	1.31217800
H	-2.73579800	-0.26133000	2.17164400
C	-2.45344400	-0.24938500	-0.00019100
C	4.06892300	-1.62482100	1.26734500
H	4.92169800	-0.93696800	1.34093000
H	4.11126900	-2.25712400	2.16171500
C	4.06914200	-1.62456200	-1.26729100
H	4.11173200	-2.25668400	-2.16177900
H	4.92190300	-0.93664700	-1.34053500
C	2.74905000	-0.83711500	1.29107400
H	1.91880000	-1.54363200	1.38784100
H	2.70528200	-0.18320300	2.16964100
C	2.74925700	-0.83693400	-1.29114700
H	2.70561000	-0.18287800	-2.16961000
H	1.91902200	-1.54343100	-1.38812600
C	4.20287800	-2.48016000	-0.00005100
H	5.16439900	-3.00516100	-0.00004400
H	3.42436000	-3.25717500	-0.00019800
C	0.58552000	3.27355300	0.00008500
H	1.06006800	4.25225400	0.00015100

Allene 10H B3LYP/6-31G*

1 1

C	-0.684672	-0.000170	-1.564042
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C	0.717422	-0.000028	-1.255733
C	1.331198	0.000000	0.000000
C	-1.765532	-0.000096	-0.705852
C	0.717422	0.000028	1.255733
C	-1.765532	0.000095	0.705852
C	-0.684672	0.000170	1.564042
H	-2.749097	-0.000134	-1.171537
H	-2.749097	0.000134	1.171537
C	1.452862	-0.000615	-2.510886
H	2.535200	-0.000434	-2.570364
C	0.591811	0.000126	-3.552046
H	0.863723	0.000785	-4.601416
C	-0.825303	0.000172	-3.070220
H	-1.386010	0.877885	-3.425412
H	-1.386645	-0.876781	-3.425992
C	-0.825303	-0.000172	3.070220
H	-1.386645	0.876782	3.425992
H	-1.386010	-0.877884	3.425412
C	1.452862	0.000615	2.510886
H	2.535200	0.000433	2.570364
C	0.591811	-0.000126	3.552046
H	0.863723	-0.000785	4.601416
H	2.419407	0.000000	0.000000

Allene 11H B3LYP/6-31G*

1	1		
C	0.008180	0.000139	-1.568730
C	-1.388938	-0.000175	-1.224916
C	-1.977347	-0.000314	0.036621
C	1.097815	0.000084	-0.729496
C	-1.343604	-0.000140	1.287340
C	1.127874	-0.000001	0.710675
C	0.049904	-0.000019	1.589376
C	-2.155462	-0.000046	-2.464871
H	-3.239042	0.000074	-2.495170
C	-1.324310	0.000121	-3.526198
H	-1.621601	0.000361	-4.568576
C	0.108271	0.000027	-3.081615
H	0.654857	-0.877565	-3.456728
H	0.654757	0.877742	-3.456605
C	0.197145	0.000072	3.095977
H	0.755084	-0.878186	3.453709
H	0.755541	0.877977	3.453784
C	-2.079477	0.000110	2.546134
H	-3.161891	0.000002	2.604690
C	-1.218803	0.000229	3.584813
H	-1.485625	0.000301	4.635339
C	2.528040	-0.000055	1.125967
H	2.852848	0.000049	2.159170
C	3.334525	-0.000291	0.046191

H	4.418388	-0.000398	0.062438
C	2.532556	0.000133	-1.220123
H	2.751857	-0.877183	-1.845929
H	2.751839	0.878039	-1.845159
H	-3.065224	-0.000449	0.056172

Allene 12H B3LYP/6-31G*

1 1			
C	-1.60189400	0.07954700	-0.00007700
C	-1.28473300	-1.30017100	0.00003400
C	-0.04040700	-1.93437800	0.00008300
C	-0.69769300	1.17391000	-0.00005700
C	1.21928700	-1.35468100	-0.00000200
C	0.71748500	1.13421800	0.00002400
C	1.57552600	0.02615600	0.00006100
C	-2.58099900	-2.07790000	0.00021200
H	-2.65620700	-2.73746000	0.87801000
C	-3.62912200	-1.01225200	-0.00016400
H	-4.69323400	-1.21721500	-0.00040700
C	-3.05552500	0.21029800	-0.00012900
C	3.03357700	0.11180100	0.00014300
C	2.49514100	-2.16764600	-0.00011100
H	2.55573200	-2.82867000	0.87746800
C	3.57029300	-1.12652400	-0.00019400
H	4.62859800	-1.36058000	-0.00044900
H	2.55566800	-2.82895200	-0.87745400
H	-2.65625900	-2.73864800	-0.87663300
H	-3.58494800	1.15443700	-0.00022200
H	3.58769100	1.04246900	0.00002000
C	-1.11360600	2.57374000	-0.00004000
H	-2.14411900	2.90463900	-0.00015500
C	-0.02947900	3.37668000	0.00002500
H	-0.03713400	4.46036100	-0.00010100
C	1.22294500	2.55971800	0.00011300
H	1.85209000	2.76896600	0.87818700
H	1.85237500	2.76901600	-0.87773300
H	-0.06503700	-3.02345300	-0.00005300

Allene 13H B3LYP/6-31G*

1 1			
C	-0.70168100	2.54773100	-0.12905000
C	-1.56388300	1.49726700	-0.20046500
C	-1.29239800	0.08509500	-0.03391100
C	0.70171400	2.54772100	0.12906900
C	-0.00000200	-0.48559200	-0.00001700
C	1.56390400	1.49724500	0.20046000
C	1.29239800	0.08508300	0.03388100
H	-1.14490300	3.53107000	-0.26434200
H	-2.59336700	1.76340500	-0.39969000

H	1.14495300	3.53105300	0.26435500
H	2.59339700	1.76336400	0.39966500
N	-2.37106300	-0.74448700	0.03489600
N	2.37105300	-0.74450300	-0.03490400
C	-3.74873300	-0.22940600	0.01811800
H	-4.01373200	0.19257100	-0.95826400
H	-4.43002700	-1.05315600	0.22368600
H	-3.89836800	0.52813100	0.79322800
C	-2.20157100	-2.19684100	0.13334800
H	-1.68326800	-2.59840900	-0.74586100
H	-1.64230400	-2.47092600	1.03573400
H	-3.18191100	-2.66650500	0.18733200
C	3.74872200	-0.22942000	-0.01810400
H	3.89837300	0.52810300	-0.79322600
H	4.01369400	0.19258000	0.95827600
H	4.43002600	-1.05317000	-0.22363800
C	2.20154700	-2.19685800	-0.13333600
H	1.68323600	-2.59841000	0.74587600
H	1.64228000	-2.47094800	-1.03572000
H	3.18188200	-2.66653500	-0.18730900
H	-0.00000500	-1.56142500	-0.00001600

Allene 14H B3LYP/6-31G*

1 1			
C	0.66586200	1.69433700	0.12741800
C	1.58754300	0.63428400	0.08326600
C	1.30860800	-0.75782700	-0.05268200
C	-0.74779300	1.66584600	0.01235900
C	0.01234900	-1.33972700	-0.05424800
C	-1.61651000	0.58340000	-0.09689300
C	-1.28717400	-0.82361400	-0.00647800
C	2.97691900	1.24307700	0.01349300
H	3.48954200	0.93346500	-0.90968000
C	2.72815600	2.71624600	0.06204100
H	3.52051300	3.45547200	0.05226300
C	1.40825100	2.95833400	0.14515600
H	0.94172300	3.93365400	0.20275300
C	-1.55708900	2.93572200	-0.14878600
H	-1.50694500	3.56489200	0.75305800
H	-1.18096500	3.55982800	-0.97219900
C	-2.95940400	1.09488100	-0.39179900
H	-3.81730800	0.47039600	-0.59830000
C	-2.94064400	2.44213800	-0.41860400
H	-3.78247300	3.09154700	-0.62699000
H	0.04658100	-2.41736300	0.02017100
H	3.63953600	0.94720800	0.83427900
N	-2.34243600	-1.70997300	0.07976500
N	2.36294700	-1.64697000	-0.15988100
C	-2.18220200	-3.11286600	-0.29044200
H	-1.70601400	-3.71306900	0.50002600

H	-3.17619100	-3.52974600	-0.47396700
H	-1.60285500	-3.20068500	-1.21237800
C	2.19804100	-2.92375500	-0.85068700
H	3.17160400	-3.22420500	-1.24946100
H	1.84365200	-3.72817700	-0.18792900
H	1.50846500	-2.81593500	-1.69031100
C	3.53461100	-1.60953000	0.72422000
H	3.71391000	-2.62177700	1.10260400
H	4.44065800	-1.27535700	0.20588500
H	3.34833200	-0.97106700	1.58779800
C	-3.44101300	-1.49909800	1.03468000
H	-4.41284500	-1.62423600	0.54509900
H	-3.36356300	-2.23875400	1.84260000
H	-3.39001000	-0.50857100	1.48340700

Allene 15H B3LYP/6-31G*

1 1			
C	-1.59548400	-0.13124100	0.23492600
C	-1.24760600	1.29325800	0.20983600
C	0.00494600	1.89987500	0.26109500
C	-0.70449300	-1.17705500	0.50623500
C	1.27309200	1.31909700	0.25528300
C	0.72983100	-1.14610200	0.60739200
C	1.61884400	-0.09385800	0.31037200
C	-2.44520700	2.04799500	0.11909400
H	-2.46795200	3.12922400	0.10017300
C	-3.53611100	1.20124600	0.03647500
C	-3.04902600	-0.18777900	0.07368600
C	3.05967300	-0.16728500	0.13789800
C	2.47332800	2.07252900	0.18705100
C	3.56157300	1.21553600	0.11507200
C	1.16381100	-2.45320100	1.11903700
H	2.17988400	-2.67620100	1.41180600
C	0.11790800	-3.27947500	1.27528800
H	0.14707800	-4.28766100	1.67187200
C	-1.13941100	-2.60156800	0.83312600
H	-1.92632400	-2.63456400	1.59702500
H	-1.53935200	-3.11308200	-0.05483500
C	-3.81491900	-1.33489800	-0.10043600
H	-3.28033500	-2.27456700	-0.12533900
C	-5.19643100	-1.47820400	-0.27581300
C	-6.21076700	-0.50212300	-0.31335900
C	-4.89763200	1.64796000	-0.06490800
C	-6.06866300	0.90028300	-0.20742200
H	2.50375800	3.15359000	0.15954100
C	4.92927600	1.63698000	0.02727600
C	6.08182100	0.86690300	-0.16035300
C	3.78343600	-1.32336500	-0.14602700
H	3.20533700	-2.23661900	-0.24410700
C	5.15239900	-1.48563500	-0.36964000

C	6.18870700	-0.52754600	-0.35743200
C	5.33316700	3.04031500	0.13369500
H	4.64402800	3.86028700	0.29190600
C	6.67266100	3.14725400	0.02427800
H	7.24926700	4.06357100	0.07502900
C	7.44929100	-1.22254500	-0.61641800
H	8.41463900	-0.73200200	-0.65834400
C	7.22577500	-2.54107400	-0.79643900
H	7.97775700	-3.29301500	-1.00640900
C	-5.26729200	3.06494700	-0.02686200
H	-4.55891800	3.87616200	0.08279100
C	-6.60410100	3.19939500	-0.13792300
H	-7.15755100	4.13122700	-0.13547600
C	-7.49110800	-1.18430000	-0.50000000
H	-8.44600000	-0.67572000	-0.56208500
C	-7.29943600	-2.51733500	-0.58409900
H	-8.07062200	-3.26601200	-0.72428900
C	-7.24380700	1.85274500	-0.26560300
H	-7.80688700	1.75575300	-1.20600900
H	-7.96881900	1.66511300	0.54072700
C	-5.84282000	-2.83781800	-0.45642100
H	-5.64442500	-3.50773300	0.39408400
H	-5.46092200	-3.36026700	-1.34694700
C	5.76464300	-2.84024600	-0.66809900
H	5.56441300	-3.57221600	0.12892200
H	5.35632600	-3.28096900	-1.59059500
C	7.27927400	1.79391400	-0.17652500
H	8.00397900	1.54786900	0.61417900
H	7.83466700	1.73337000	-1.12443200
H	-0.00789500	2.98899000	0.25079600

Allene 16H B3LYP/6-31G*

1 1			
C	1.58363200	0.36171800	0.00012100
C	1.24798200	-1.08545000	0.00012300
C	-0.01624000	-1.67555500	0.00011900
C	0.73461400	1.43105100	0.00013300
C	-1.26668800	-1.06235000	0.00012400
C	-0.72760400	1.45136200	0.00011900
C	-1.60056800	0.38337700	0.00014400
C	2.45285500	-1.82576800	0.00010000
H	2.49493100	-2.90973600	0.00008100
C	3.53613600	-0.93833600	0.00009200
C	3.04029100	0.41092100	0.00011000
C	-3.05370200	0.43487900	0.00015800
C	-2.47725400	-1.80445800	0.00013600
H	-2.51970200	-2.88830200	0.00018400
C	-3.55172000	-0.91743400	0.00017100
C	-1.12752700	2.85743600	0.00010000
H	-2.15592000	3.19041500	0.00006900

C	-0.05190400	3.66555500	0.00005500
H	-0.07542400	4.74957800	-0.00006300
C	1.22038000	2.87036800	0.00008500
H	1.84380200	3.08896800	0.87936400
H	1.84376300	3.08888900	-0.87927100
C	4.11271100	1.29657300	0.00001000
H	4.08855500	2.37842200	0.00009700
C	-4.13777900	1.31205200	-0.00003500
H	-4.12863300	2.39399800	-0.00001700
C	-5.33644300	0.54590300	-0.00006900
C	-4.97926200	-0.89017300	0.00006900
C	4.95957600	-0.90667900	0.00000600
C	5.31669600	0.53193100	-0.00005800
C	-5.82669100	-1.98674900	0.00006400
H	-5.34036800	-2.96069200	0.00019300
C	5.81390000	-2.00202400	-0.00003400
H	5.33044300	-2.97743900	0.00002900
C	7.21434400	-2.02178500	-0.00013600
H	7.66918400	-3.00893600	-0.00014500
C	8.10198200	-0.94462500	-0.00021800
H	9.15659700	-1.21101600	-0.00028400
C	-7.23060100	-2.01164200	-0.00010300
H	-7.68080300	-3.00096200	-0.00008100
C	-8.11953800	-0.94006900	-0.00027300
H	-9.17371500	-1.20796800	-0.00037000
C	-6.62516200	1.09447900	-0.00019600
H	-6.66913500	2.18228500	-0.00024100
C	-7.85323700	0.43918000	-0.00030600
H	-8.72854800	1.08377900	-0.00043500
C	6.60038600	1.08311400	-0.00016600
H	6.64176400	2.17105900	-0.00020900
C	7.83369900	0.43056300	-0.00022900
H	8.70656300	1.07837800	-0.00030400
H	-0.02692100	-2.76490200	0.00010400

Allene 17H B3LYP/6-31G*

1 1			
C	-1.58630600	-0.83372200	-0.00026700
C	-1.25037400	0.61124300	-0.00028800
C	0.01371300	1.19944900	-0.00030300
C	-0.73490200	-1.90329500	-0.00021400
C	1.26524600	0.58776400	-0.00022700
C	0.72448500	-1.92357800	-0.00018900
C	1.59951800	-0.85579000	-0.00019700
C	-2.45914200	1.34987700	-0.00026900
H	-2.49251100	2.43328300	-0.00029900
C	-3.54482600	0.46679000	-0.00024700
C	-3.04025300	-0.88359900	-0.00025100
C	3.05140500	-0.90752000	-0.00007900
C	2.47830900	1.32825000	-0.00019600

H	2.51110400	2.41150400	-0.00027100
C	3.55708000	0.44625100	-0.00007800
C	1.12491800	-3.33075600	-0.00021500
H	2.15372100	-3.66262100	-0.00019200
C	0.04999700	-4.13925500	-0.00015300
H	0.07327400	-5.22336000	-0.00018600
C	-1.22159900	-3.34228100	-0.00009900
H	-1.84615300	-3.55952300	0.87895800
H	-1.84643100	-3.55966500	-0.87890700
C	-4.10577700	-1.77285800	-0.00014000
H	-4.07655300	-2.85473000	-0.00016600
C	4.12833300	-1.78751300	-0.00002300
H	4.11514300	-2.86958900	-0.00003400
C	5.33394700	-1.02716500	0.00011500
C	4.99091300	0.40798600	-0.00002800
C	-4.97550800	0.42265900	-0.00011600
C	-5.31651000	-1.01503200	-0.00006700
C	5.86412100	1.48721700	-0.00001000
C	6.61042000	-1.60391300	0.00023500
H	6.62697200	-2.69362600	0.00028800
C	-5.85579000	1.49958800	-0.00003100
C	-6.58876900	-1.59517200	0.00005400
H	-6.60202800	-2.68494800	0.00007400
C	7.29058400	1.50258400	0.00006200
C	8.17153600	0.40651700	0.00013800
C	7.84785200	-0.98142800	0.00023300
C	-7.27948300	1.50934800	0.00008900
C	-8.15781100	0.40805000	0.00017500
C	-7.83039400	-0.97641300	0.00017200
C	9.63042600	0.51958600	0.00018900
H	10.16731800	1.46011700	0.00015700
C	10.19807500	-0.70314600	0.00031800
H	11.26193700	-0.91086900	0.00035000
C	-7.71807500	2.90797800	0.00011800
H	-8.75597000	3.21731000	0.00023700
C	-6.65740300	3.73551100	0.00001100
H	-6.68927700	4.81868900	-0.00001800
C	-9.61708800	0.51762100	0.00031600
H	-10.15654900	1.45664500	0.00032600
C	-10.18110900	-0.70693800	0.00052900
H	-11.24424800	-0.91825100	0.00066300
C	9.14498500	-1.76796200	0.00025400
H	9.22204200	-2.42675900	0.87822600
H	9.22212700	-2.42664000	-0.87782500
C	-9.12420700	-1.76755300	0.00034500
H	-9.19902500	-2.42667700	0.87831400
H	-9.19930500	-2.42656700	-0.87770700
C	-5.38358500	2.94186200	-0.00006800
H	-4.76051800	3.15873100	-0.87957600
H	-4.76039500	3.15872100	0.87934000
C	5.38652200	2.92796400	0.00001500
H	4.76272400	3.14301700	-0.87948300

H	4.76265000	3.14296300	0.87945700
C	7.72217300	2.90288800	0.00006800
H	8.75861700	3.21709600	0.00013900
C	6.65783400	3.72580600	0.00005700
H	6.68570200	4.80913900	0.00005900
H	0.02473800	2.28921300	-0.00034800

Allene 18H B3LYP/6-31G*

1 1

C	-1.58748300	-1.01086400	-0.01988400
C	-1.25372000	0.43496400	-0.02091400
C	0.01486100	1.02027200	-0.02576400
C	-0.73351200	-2.07698400	-0.02567400
C	1.26194300	0.40608100	-0.02554700
C	0.72522500	-2.11249900	-0.02956700
C	1.60046300	-1.03239100	-0.02100100
C	-2.46388800	1.16695500	-0.01877200
H	-2.49799300	2.25088100	-0.02039300
C	-3.55132400	0.28219900	-0.01555800
C	-3.04235300	-1.06559900	-0.01661300
C	3.04252700	-1.08396500	-0.01014500
C	2.48055900	1.15147400	-0.02488400
H	2.50872700	2.23522500	-0.02748200
C	3.55432000	0.27176900	-0.01590900
C	1.12291900	-3.49714000	-0.05115600
H	2.15116700	-3.82158600	-0.08570800
C	0.03090800	-4.32965800	-0.04223500
C	-1.23658500	-3.50782800	-0.03562000
H	-1.85995800	-3.72227200	0.84406400
H	-1.86297000	-3.70353800	-0.91720200
C	-4.10872900	-1.95621400	-0.01408600
H	-4.07932100	-3.03868300	-0.01341000
C	4.12485300	-1.96299500	0.01091400
H	4.11029800	-3.04547500	0.02827800
C	5.33044500	-1.20590300	0.01580500
C	4.99543700	0.22530300	-0.00300600
C	-4.98361000	0.23206300	-0.01192100
C	-5.32146900	-1.20126000	-0.01083300
C	5.87071100	1.29875700	-0.00875500
C	6.61405800	-1.77616600	0.03708800
H	6.63579300	-2.86628000	0.05288400
C	-5.87008000	1.30530400	-0.00784100
C	-6.59810600	-1.77550700	-0.00506000
H	-6.61624300	-2.86590000	-0.00230800
C	7.29676200	1.33647000	-0.00008600
C	8.18601300	0.23637000	0.02447600
C	7.84385200	-1.14904500	0.04031100
C	-7.28914600	1.33653200	-0.00267600
C	-8.17810500	0.22759600	-0.00240200
C	-7.83401300	-1.15288200	-0.00286900

C	9.62405500	0.35653800	0.04580100
H	10.15244800	1.29913500	0.05917600
C	10.21353200	-0.88544400	0.05869100
C	-7.72940200	2.71693400	0.01017300
H	-8.76615000	3.02071500	0.03086900
C	-6.65209800	3.56342900	-0.00081600
C	-9.61424900	0.34852000	0.00628500
H	-10.14367300	1.29026700	0.02328600
C	-10.20312100	-0.89580200	-0.00232000
C	9.13708600	-1.94531800	0.07141100
H	9.19298700	-2.57793700	0.96830100
H	9.21751800	-2.61908300	-0.79308800
C	-9.12431100	-1.95281600	0.00655100
H	-9.18830400	-2.59682600	0.89479600
H	-9.19626200	-2.61544900	-0.86726400
C	-5.38208400	2.74243100	0.00022000
H	-4.75758800	2.95540800	-0.87756600
H	-4.76148300	2.93873800	0.88462100
C	5.37586400	2.73360400	-0.03899400
H	4.76073000	2.91663300	-0.93022400
H	4.74342200	2.95512600	0.83128200
C	7.72533300	2.71878600	-0.02855900
H	8.76024700	3.02928700	-0.04791900
C	6.64283500	3.55917100	-0.03833500
H	0.02745500	2.11061100	-0.02812400
N	0.02403700	-5.68881700	-0.00645000
C	1.29360900	-6.39847300	-0.07797500
H	1.13028500	-7.45221500	0.15903100
H	1.75122300	-6.32876600	-1.07588300
H	1.99241300	-5.98493900	0.65568100
C	-1.17612900	-6.45651500	-0.31050600
H	-1.14606900	-7.40589500	0.23259000
H	-2.06635500	-5.91356600	0.01015600
H	-1.26902700	-6.67655100	-1.38501600
N	-11.52846600	-1.19140900	-0.04820300
N	-6.64973600	4.92726200	-0.05383700
N	6.63437900	4.92358200	-0.00385400
N	11.54139600	-1.18174900	0.02565000
C	-12.49255100	-0.10207800	0.02476400
H	-12.52471800	0.35616100	1.02421600
H	-12.23587400	0.67154300	-0.70551900
H	-13.48656500	-0.48462200	-0.21682000
C	-12.01701700	-2.53266600	0.24420200
H	-11.31554600	-3.28258400	-0.12573200
H	-12.16815800	-2.69672800	1.32206400
H	-12.97297300	-2.68734500	-0.26390800
C	-7.92520900	5.62253900	0.03164700
H	-7.77629400	6.67916500	-0.20247400
H	-8.62431100	5.20451800	-0.69946700
H	-8.37790400	5.54373300	1.03199800
C	-5.45950100	5.68675900	0.30202800
H	-4.56386400	5.18587000	-0.07114500

H	-5.51011700	6.67445400	-0.16498100
H	-5.35447100	5.82438100	1.38994200
C	5.44491800	5.67455800	-0.37972400
H	5.48363700	6.66502900	0.08277300
H	5.35444400	5.80612400	-1.46968600
H	4.54712100	5.17036000	-0.01666400
C	7.90725900	5.62402100	-0.08565800
H	8.36842200	5.53780200	-1.08150600
H	7.75136600	6.68218300	0.13694700
H	8.60234500	5.21643100	0.65503300
C	12.02710800	-2.51299700	0.36378500
H	11.33327400	-3.27449800	0.00301200
H	12.99163600	-2.67961200	-0.12416400
H	12.16105300	-2.64802100	1.44822400
C	12.50190600	-0.08982700	0.09474000
H	13.49875400	-0.47223000	-0.13590400
H	12.24835800	0.67530800	-0.64553900
H	12.52639600	0.38004700	1.08937500

Allene 19H B3LYP/6-31G*

1 1

C	1.59235700	0.95558600	-0.08535200
C	1.24923100	-0.49063500	-0.06805000
C	-0.00992800	-1.08230800	-0.00704100
C	0.72015900	2.03303300	-0.04466600
C	-1.26372100	-0.47184700	0.05374900
C	-0.71102500	2.05230900	0.02495200
C	-1.60507500	0.97506000	0.07009200
C	2.45546500	-1.23291900	-0.12550500
H	2.48669500	-2.31655200	-0.12443400
C	3.53908100	-0.34963000	-0.17693700
C	3.01723700	1.00499900	-0.15299400
C	-3.02714500	1.02711900	0.13966700
C	-2.46758100	-1.21450300	0.11261800
H	-2.49914400	-2.29779500	0.11202100
C	-3.54955200	-0.32912000	0.16464400
C	-1.12386700	3.45885600	0.04265700
H	-2.15454200	3.78216300	0.09084100
C	-0.05528100	4.27397000	-0.01029200
H	-0.07831500	5.35788100	-0.01133200
C	1.20995000	3.46969300	-0.07005700
H	1.87765700	3.68573100	0.77717700
H	1.79286900	3.68351000	-0.97823500
C	4.10124600	1.89065900	-0.20857800
H	4.07484800	2.97297600	-0.21849500
C	-4.12225800	1.90912500	0.19855100
H	-4.10831700	2.99134300	0.21117200
C	-5.30874700	1.15333400	0.24420400
C	-4.96660200	-0.28333800	0.22678800
C	4.95800100	-0.29753000	-0.23640000

C	5.29536400	1.13412800	-0.25259800
C	-5.85290800	-1.36526700	0.33583900
C	-6.60341500	1.72072800	0.31371900
H	-6.62507000	2.80905000	0.36315700
C	5.85055000	-1.37893500	-0.34640500
C	6.58786200	1.70769100	-0.31824400
H	6.60501100	2.79601700	-0.36814800
C	-7.26538000	-1.39398200	0.34250600
C	-8.17285000	-0.29715000	0.16097900
C	-7.82595000	1.09880700	0.27178300
C	7.25986000	-1.40266300	-0.34567000
C	8.16561000	-0.30257100	-0.15345100
C	7.81317300	1.09110400	-0.26889800
C	-9.57555500	-0.40029900	-0.10953700
C	-10.19729900	0.89245400	0.02216100
C	7.67584800	-2.78219100	-0.63404900
H	8.70045000	-3.08849400	-0.79624600
C	6.60483700	-3.59121600	-0.74622100
H	6.62195400	-4.64965900	-0.97793600
C	9.56438600	-0.40194100	0.12744700
C	10.18363800	0.89355300	0.00151500
C	-9.10770000	1.90366200	0.27863200
H	-9.25788700	2.40960600	1.24316500
H	-9.11266800	2.69107000	-0.48667800
C	9.09210600	1.90046100	-0.26670800
H	9.08612800	2.69033800	0.49590100
H	9.24802200	2.40381400	-1.23166300
C	5.35223200	-2.79817800	-0.54129900
H	4.67069400	-2.87741100	-1.39968300
H	4.78393900	-3.14513700	0.33484200
C	-5.34940300	-2.78492000	0.51763300
H	-4.78625700	-3.12427200	-0.36479500
H	-4.66146800	-2.86813700	1.37049500
C	-7.67332700	-2.77650200	0.62509800
H	-8.69513500	-3.08856700	0.79386100
C	-6.59863700	-3.58232100	0.72607700
H	-6.61130700	-4.64193000	0.95279400
C	-10.24884600	-1.56518800	-0.60938700
H	-9.60448300	-2.38681500	-0.90187200
C	10.23827600	-1.56671200	0.63001400
H	9.59415200	-2.39100600	0.91592500
C	11.57513300	-1.77357500	0.84638600
H	11.83663400	-2.75270400	1.24192800
C	12.68586500	-0.89573500	0.63415200
H	13.66715700	-1.33292800	0.80045300
C	-11.58754900	-1.77656800	-0.81539500
H	-11.84840200	-2.75627400	-1.20987900
C	-12.69865100	-0.90415200	-0.59255700
H	-13.67982600	-1.34404500	-0.75215600
C	-11.52263700	1.24896800	-0.03175100
H	-11.73821000	2.30162400	0.14121200
C	-12.66411900	0.42367700	-0.25624100

H	-13.62385700	0.92886200	-0.17409700
C	11.50630400	1.25464500	0.06734800
H	11.72025000	2.30814000	-0.10257000
C	12.64947200	0.43180100	0.30055300
H	13.60808100	0.94045800	0.22657900
H	-0.01908500	-2.17202600	-0.00620600

M052X

Neutral

Allene 1 M052X/6-31G*

0 1			
C	0.69550400	1.27831200	0.21442100
C	1.60074200	0.26468500	0.18654200
C	1.22053800	-1.03604500	-0.35973100
C	-0.69564900	1.27823900	-0.21440300
C	0.00004200	-1.39023700	-0.00008400
C	-1.60079200	0.26453100	-0.18655900
C	-1.22039800	-1.03613600	0.35980000
H	1.06229000	2.24823500	0.53618400
H	2.61892100	0.45786400	0.51087800
H	1.84258900	-1.57590100	-1.06363100
H	-1.06251100	2.24811400	-0.53623400
H	-2.61895900	0.45756400	-0.51101700
H	-1.84224100	-1.57596100	1.06390600

Allene 2 M052X/6-31G*

0 1			
C	0.36457900	-0.61066000	-0.10409600
C	0.54038500	0.75632800	-0.11387400
C	-0.56871700	1.64729500	-0.42917800
C	-0.82816300	-1.39029100	-0.33625300
C	-1.70600600	1.23015600	0.10159200
C	-2.12362600	-1.04807300	-0.09002100
C	-2.44274000	0.22658500	0.54721700
H	-0.47403900	2.47050600	-1.12782400
H	-0.65111100	-2.39793500	-0.70293200
H	-2.90449000	-1.77068100	-0.30638600
H	-3.14085800	0.29575000	1.37374600
C	1.95741600	1.06548000	0.10436100
H	2.35730700	2.06894600	0.14744500
C	2.64943100	-0.07907900	0.22666300
H	3.71308700	-0.17278300	0.39293100
C	1.71912300	-1.25060400	0.09446900
H	1.74520900	-1.89544100	0.97976200
H	1.98479700	-1.88118800	-0.76202300

Allene 3 M052X/6-31G*

0 1

C	-0.75859700	-0.03502400	-0.18586000
C	-1.42836900	1.15805600	-0.02781000
C	-2.86110000	1.25312000	-0.27818600
C	-1.27875700	-1.33521000	-0.53475800
C	-3.51084700	0.19494500	0.17566600
C	-2.51364500	-1.85294600	-0.27891200
C	-3.49345600	-1.09049600	0.48791700
H	-3.29832700	2.04222000	-0.87903200
H	-0.56788400	-2.00566100	-1.00976900
H	-2.72602800	-2.87093100	-0.59139800
H	-4.06139600	-1.53521000	1.29723300
C	-0.46388400	2.21270700	0.29593900
H	-0.73305500	3.24434800	0.47634300
C	0.77146500	1.68974300	0.32226300
H	1.68289400	2.23248000	0.52930900
C	0.73170600	0.21452700	-0.00188200
C	1.51517600	-0.07701400	-1.30364000
H	1.13080600	0.56223300	-2.10194400
H	1.33086200	-1.11582600	-1.59836900
C	1.30113900	-0.64669200	1.14728700
H	0.76632600	-0.40793500	2.06945200
H	1.09582600	-1.69825900	0.91802400
C	3.02340300	0.11277600	-1.12390300
H	3.53453200	-0.13478300	-2.05755900
H	3.24291200	1.16423000	-0.91397400
C	2.80955800	-0.45993600	1.32159100
H	3.16820500	-1.11441600	2.11985900
H	3.02214100	0.56672200	1.63699500
C	3.55243900	-0.75741000	0.01764700
H	3.40843000	-1.81257800	-0.24230300
H	4.62636500	-0.60351300	0.14697500

Allene 4 M052X/6-31G*

0 1

C	-0.53144900	0.64463600	0.27348100
C	-0.44533700	-0.78080500	-0.01724700
C	0.70891500	-1.38198200	0.26581300
C	0.52767500	1.47431900	0.08191500
C	2.00221100	-1.17054500	0.45386300
C	1.85906300	1.12451600	-0.38148800
C	2.54574400	-0.04717800	-0.30578700
H	2.60203600	-1.69884500	1.18819300
H	3.53589800	-0.09888600	-0.74929000
C	-1.77645900	-1.20277800	-0.46949400
H	-2.00601600	-2.18470000	-0.85700000
C	-2.65566100	-0.21773600	-0.23176700
H	-3.72184500	-0.28061900	-0.40067800
C	-1.99680200	1.00689800	0.37751200
H	-2.33150200	1.14690000	1.41213500
H	-2.22288700	1.92856800	-0.16365900

H	0.33560800	2.54117800	0.14512900
H	2.38129400	1.95034000	-0.85563800

Allene 5 M052X/6-31G*

0 1			
C	-0.68232500	-0.17379200	0.03869500
C	-1.38961200	1.06236700	-0.27241300
C	-2.62174600	1.19319600	0.21426600
C	-1.33667900	-1.36361700	0.09407200
C	-3.67106800	0.51860500	0.65712700
C	-2.75387000	-1.61233400	-0.11505700
C	-3.83305200	-0.80246200	0.05423000
H	-0.73254100	-2.26242400	0.16379400
H	-4.29984900	0.84614200	1.47889700
H	-2.96801600	-2.62260900	-0.45153700
H	-4.81803600	-1.19033300	-0.18868900
C	-0.44022400	1.91797300	-0.99150100
H	-0.69604700	2.85934700	-1.45613900
C	0.78815800	1.38992100	-0.88810600
H	1.68672400	1.85263900	-1.27266400
C	0.81030000	0.08307000	-0.09722100
C	1.55052200	-1.04554900	-0.83393000
H	1.10310200	-1.18955000	-1.82027200
H	1.41084000	-1.97619000	-0.27265500
C	1.46328200	0.30086100	1.28937700
H	0.94972900	1.11815800	1.80130900
H	1.30387100	-0.60774800	1.88086500
C	3.05351400	-0.77445100	-0.94468300
H	3.22846000	0.10850500	-1.56776800
H	3.53853500	-1.61377700	-1.44888100
C	3.67397000	-0.55583500	0.43694900
C	2.96442300	0.57600100	1.18288300
H	3.13081400	1.52198300	0.65753900
H	3.38712300	0.69405600	2.18352600
H	4.74151100	-0.34229600	0.34506400
H	3.58021200	-1.47963300	1.01948200

Allene 6 M052X/6-31G*

0 1			
C	-0.70384700	-0.45203600	-0.05376200
C	-1.58189400	0.58999800	0.17095100
C	-1.12445000	1.89574800	0.60235300
C	0.73542700	-0.43890900	0.01705200
C	-0.00606100	2.27647400	-0.00072100
C	1.60126700	0.61548900	-0.18296200
C	1.11863200	1.92511800	-0.60322900
H	-1.59965600	2.43739400	1.41344800
H	1.58107100	2.47501500	-1.41558400
C	-2.99536900	0.08980100	0.04633300
H	-3.56663800	0.26283000	0.96585800

C	-2.81494400	-1.37253800	-0.24783800
H	-3.63243900	-2.06145200	-0.40440800
C	-1.50678000	-1.66616500	-0.29582800
H	-1.08247400	-2.64069400	-0.49571000
C	1.56092800	-1.67716800	0.27924600
H	1.31107600	-2.14555200	1.23733600
H	1.39422500	-2.43554200	-0.49473000
C	2.98103800	0.14216600	-0.02717400
H	3.85091100	0.77623400	-0.12828000
C	2.97556200	-1.17321400	0.24220000
H	3.84019000	-1.80198300	0.39953400
H	-3.53332100	0.60515900	-0.75718900

Allene 7 M052X/6-31G*

0 1

C	1.20506600	0.83527800	-0.10242200
C	1.50461200	2.18360500	-0.08935600
C	0.50098900	3.20893300	-0.35421300
C	-0.10504700	0.22285000	-0.19894500
C	-0.63059300	2.96490400	0.28128700
C	-1.32023600	0.76048900	0.19175400
C	-1.43779600	2.05953900	0.81790800
H	0.65544700	4.00312600	-1.07586300
H	-2.04697500	2.22875600	1.69961000
C	2.93704400	2.36528000	0.14957200
H	3.41796700	3.33130500	0.21924400
C	3.52250900	1.16564300	0.26209200
H	4.57568400	0.98756600	0.42620700
C	2.51625600	0.05969200	0.03592000
C	2.90556600	-0.65225600	-1.28963700
H	3.00513600	0.10458400	-2.07120900
H	2.10552900	-1.32543400	-1.59830300
C	2.47644700	-0.94586600	1.20469200
H	2.27741800	-0.40060600	2.13036200
H	1.63734700	-1.63185800	1.05107600
C	4.19183300	-1.47141000	-1.15040700
H	4.38964700	-1.99307900	-2.09017400
H	5.04398900	-0.80787200	-0.97448100
C	3.76811400	-1.75875400	1.31619300
H	3.67287000	-2.48357800	2.12844800
H	4.60208700	-1.09977200	1.57878400
C	4.08106100	-2.47324400	0.00041000
H	3.27650700	-3.18508500	-0.21977800
H	5.00359400	-3.05177100	0.09035600
C	-2.44333200	-0.22566900	-0.02180900
C	-0.38924000	-1.16543700	-0.63121900
H	0.35229800	-1.86965400	-0.97404400
C	-1.70126100	-1.42654200	-0.54487700
H	-2.17250800	-2.36243600	-0.81044300
C	-3.44575800	0.33744000	-1.05621800
H	-2.92009100	0.51917900	-1.99643400

C	-3.18351500	-0.53054900	1.29862200
H	-2.47779100	-0.95595300	2.01595800
C	-4.37935700	-1.46158500	1.08513700
H	-4.02925300	-2.43935800	0.73884800
H	-4.88726700	-1.62847600	2.03826100
C	-4.64313800	-0.59094700	-1.26498000
H	-5.33751500	-0.13763600	-1.97675600
H	-4.30587600	-1.53349800	-1.70877100
C	-5.35255200	-0.87691400	0.05983000
H	-5.76607000	0.05876500	0.45325900
H	-6.19297600	-1.55733400	-0.09715000
H	-3.79813300	1.30739200	-0.68816100
H	-3.54709400	0.41583700	1.71516200

Allene 8 M052X/6-31G*

0 1

C	-0.80217600	-0.46175700	-0.33891000
C	-1.50762900	0.74887800	0.05371500
C	-0.93923100	1.92354800	-0.22381400
C	0.55697600	-0.54005100	-0.26384500
C	0.22884300	2.49831700	-0.47396000
C	1.51060100	0.50763700	0.13885400
C	1.39683700	1.85952500	0.12359700
H	0.35221800	3.32167400	-1.17144200
H	2.24236000	2.45414100	0.46161300
C	-2.80306400	0.32709200	0.60178700
H	-3.51493100	0.99794200	1.06058800
C	-2.98868100	-0.97657000	0.34963200
H	-3.88651600	-1.53453700	0.57720100
C	-1.80055700	-1.59931100	-0.36004200
H	-2.07667300	-1.91969500	-1.37168200
H	-1.41648000	-2.47872800	0.16344700
C	2.80855200	-0.19251000	0.51867300
H	3.67751800	0.26209100	0.03526100
H	2.97888500	-0.13629300	1.59990800
C	1.32597100	-1.79103100	-0.34576100
H	0.90264100	-2.72431700	-0.69097700
C	2.58022300	-1.61411200	0.08556500
H	3.34099000	-2.38021700	0.14313300

Allene 9 M052X/6-31G*

0 1

C	-1.16471600	0.77810200	-0.11337100
C	-1.31278300	2.12091200	0.43002300
C	-0.46486100	3.07126900	0.03170800
C	0.07054400	0.29164900	-0.44861300
C	0.74034000	3.27211200	-0.47312000
C	1.38642200	0.93252500	-0.23720100
C	1.72656500	2.24236400	-0.15219200
H	0.97283000	4.05590500	-1.18801000

H	2.76241900	2.50915400	0.03705600
C	-2.54793200	2.14459200	1.21578700
H	-2.87595800	2.98938800	1.80451700
C	-3.23590900	1.02069800	0.98146500
H	-4.22129800	0.81140100	1.37399000
C	-2.49070300	0.03823200	0.08317500
C	0.37387100	-1.08433600	-0.87925500
H	-0.36580300	-1.76800900	-1.26832300
C	1.67565400	-1.35669900	-0.74647000
H	2.13862500	-2.30033000	-0.99972100
C	3.91742300	-1.52882600	1.40002500
H	4.20087200	-1.65021500	2.44843300
H	3.49512500	-2.48509700	1.07402200
C	5.14697000	-1.19670700	0.55239200
H	5.89118200	-1.99281300	0.63088800
H	5.61122700	-0.28347100	0.94225200
C	4.75867600	-0.97168100	-0.91027800
H	5.63777000	-0.69425300	-1.49699100
H	4.38297100	-1.90720700	-1.33650000
C	2.85969000	-0.43037700	1.27778500
H	1.96847200	-0.67601900	1.86051500
H	3.26359800	0.50622600	1.67843800
C	3.69888500	0.12711100	-1.03141000
H	4.14154100	1.06402200	-0.68012400
H	3.40700500	0.27886600	-2.07345800
C	2.44395100	-0.17965600	-0.19187300
C	-4.56381400	-0.89398900	-1.08377700
H	-5.25171300	-0.26303400	-0.51181600
H	-5.02444000	-1.05437600	-2.06155300
C	-3.68887800	-2.02336700	0.99339600
H	-3.52627800	-2.98590200	1.48459100
H	-4.34638300	-1.44536900	1.64977700
C	-3.22571600	-0.17343300	-1.25893200
H	-2.58019300	-0.77207700	-1.91166300
H	-3.36456300	0.79547400	-1.74433200
C	-2.34336900	-1.30909000	0.82581400
H	-1.87400900	-1.12753700	1.79577500
H	-1.67778500	-1.96933100	0.26832900
C	-4.37361900	-2.22809900	-0.35991500
H	-5.33444000	-2.73115300	-0.22751100
H	-3.75090800	-2.88408700	-0.97956000

Allene 10 M052X/6-31G*

0 1			
C	-1.55595100	0.60179700	0.32903600
C	-1.23498000	-0.73894600	-0.13813100
C	0.00000200	-1.24800500	0.00001800
C	-0.68939600	1.64478000	0.21599200
C	1.23498900	-0.73894800	0.13813700
C	0.68938600	1.64478200	-0.21597300
C	1.55594300	0.60180300	-0.32902300

H	-1.09600300	2.63353400	0.40794800
H	1.09598800	2.63353700	-0.40793400
C	-2.49774500	-1.32682200	-0.60601100
H	-2.56713400	-2.28377200	-1.10298700
C	-3.52357200	-0.55068200	-0.22527300
H	-4.57026500	-0.78086500	-0.36939700
C	-3.05498000	0.68864900	0.51241800
H	-3.45727900	1.61411200	0.09338800
H	-3.36228700	0.64822700	1.56428500
C	3.05497000	0.68866100	-0.51243000
H	3.36225100	0.64825500	-1.56430500
H	3.45727800	1.61411700	-0.09339400
C	2.49775700	-1.32679700	0.60603800
H	2.56715300	-2.28373300	1.10304000
C	3.52358000	-0.55069400	0.22521300
H	4.57027600	-0.78089000	0.36929800

Allene 11 M052X/6-31G*

0 1

C	-1.56456700	-0.05185100	0.29278900
C	-1.20858800	-1.39330600	-0.15199500
C	0.03093900	-1.88973500	-0.00902500
C	-0.70957400	0.99872000	0.19542900
C	1.26006400	-1.36307900	0.14044200
C	0.70030900	1.01344800	-0.20803600
C	1.58707000	-0.02089300	-0.30678000
C	-2.45478000	-2.01800700	-0.61845600
H	-2.49512600	-2.98755600	-1.09372600
C	-3.50228900	-1.26089900	-0.26255900
H	-4.54222900	-1.51836400	-0.40914100
C	-3.06938600	0.01127900	0.43969500
H	-3.48325500	0.90821900	-0.02887800
H	-3.40138900	0.01658700	1.48486700
C	3.09224600	0.08401900	-0.42993800
H	3.44475500	0.10074000	-1.46820800
H	3.47212600	0.98791700	0.05344800
C	2.51508900	-1.96076700	0.61827700
H	2.57289500	-2.92987100	1.09270500
C	3.54787900	-1.17796700	0.27483100
H	4.59214200	-1.41111000	0.43117500
C	1.06857900	2.42766400	-0.37796200
H	2.04381500	2.74715800	-0.71778200
C	0.05300000	3.23406900	-0.05053800
H	0.06931400	4.31456800	-0.08319500
C	-1.14981000	2.44151300	0.37773300
H	-2.03160900	2.68230000	-0.22515100
H	-1.41852500	2.64416900	1.42044500

Allene 12 M052X/6-31G*

0 1

C	1.58695200	0.01569000	-0.31075400
C	1.27250800	-1.32270200	0.14216000
C	0.04286700	-1.83933600	-0.00426100
C	0.68557900	1.05336500	-0.21311400
C	-1.20297600	-1.36890700	-0.14403100
C	-0.70466800	1.02672200	0.21229400
C	-1.56049100	-0.03688900	0.30816000
C	2.56271900	-1.96089000	0.62220200
H	2.68279500	-2.96662900	0.21721900
C	3.60392100	-0.99115800	0.11111700
H	4.66652000	-1.15655700	0.22675200
C	3.04777600	0.10201600	-0.43515300
C	-3.02402100	0.00042100	0.44095900
C	-2.47390900	-2.04146500	-0.62956700
H	-2.52212600	-2.11442700	-1.72300700
C	-3.54426800	-1.10796800	-0.10944700
H	-4.60124200	-1.30958800	-0.22007300
H	-2.56546700	-3.05426200	-0.23465900
H	2.61256700	-2.04356100	1.71497300
H	3.59037800	0.94886900	-0.83169700
H	-3.58918400	0.82716100	0.84905400
C	1.04339100	2.46819900	-0.38878300
H	2.01564100	2.79556000	-0.72927200
C	0.02292900	3.26816100	-0.05715500
H	0.02937700	4.34854900	-0.09161500
C	-1.16485500	2.46325800	0.38808700
H	-2.05738600	2.68219100	-0.20724100
H	-1.42259900	2.67159500	1.43293200

Allene 13 M052X/6-31G*

0 1

C	0.47311900	2.26452800	0.54747300
C	1.22665100	1.23382000	1.01020200
C	1.20087600	-0.06755700	0.35113300
C	-0.47343300	2.26460000	-0.54713100
C	0.00008700	-0.54636900	-0.00033300
C	-1.22681900	1.23392100	-1.01015100
C	-1.20087700	-0.06756300	-0.35125000
H	0.62919200	3.23246900	1.01339200
H	1.91777100	1.41506100	1.82928100
H	-0.62957200	3.23262600	-1.01285800
H	-1.91783700	1.41522800	-1.82930000
N	2.40462700	-0.75937800	0.18857600
N	-2.40444900	-0.75947700	-0.18838200
C	3.58533000	0.01294000	-0.16188200
H	4.47600600	-0.57885300	0.05509400
H	3.59874800	0.28319700	-1.22702300
H	3.63232100	0.92801900	0.42319200
C	2.30834600	-2.00126900	-0.55188300
H	3.24889800	-2.54506900	-0.45057200
H	1.49255600	-2.59495000	-0.14108000

H	2.10666100	-1.83817600	-1.61903900
C	-3.58548900	0.01254500	0.16150700
H	-3.63239400	0.92763900	-0.42354300
H	-4.47593000	-0.57943800	-0.05591800
H	-3.59949000	0.28275500	1.22665000
C	-2.30800000	-2.00130900	0.55213100
H	-3.24843000	-2.54530700	0.45074700
H	-1.49203400	-2.59482500	0.14142700
H	-2.10646300	-1.83812300	1.61929700

Allene 14 M052X/6-31G*

O 1			
C	0.31335600	1.61231200	-0.31275000
C	1.39435700	0.75490500	-0.39372600
C	1.38662400	-0.56221300	0.21423700
C	-0.97108600	1.37148900	0.28193100
C	0.24204300	-1.26284200	0.14306100
C	-1.61030800	0.17277100	0.49330100
C	-1.07242200	-1.07642800	-0.02400100
C	2.57488400	1.51380000	-0.94508000
H	3.39538800	1.51867800	-0.21811800
C	2.02642900	2.89102100	-1.18301100
H	2.60112300	3.70386400	-1.60305200
C	0.73976500	2.93290000	-0.81020100
H	0.08805000	3.79439700	-0.86565800
C	-1.86330500	2.47541400	0.80297200
H	-1.35824900	3.08714000	1.55823800
H	-2.16625300	3.15584400	-0.00167900
C	-2.88604000	0.41674000	1.17782000
H	-3.56755600	-0.36973900	1.47117800
C	-3.04525400	1.73669800	1.36536200
H	-3.88471900	2.22250300	1.84164300
H	2.96430800	1.06724300	-1.86665900
N	2.54183500	-0.99039800	0.92729400
N	-1.93560400	-2.00333800	-0.61552600
C	3.59288900	-1.47199000	0.03484200
H	4.49387500	-1.67426200	0.61668800
H	3.28846700	-2.39368700	-0.48331100
H	3.83206900	-0.72118500	-0.71591300
C	2.22170000	-2.01105800	1.91054400
H	1.81685300	-2.92085100	1.44279100
H	3.12877900	-2.26321800	2.46177700
H	1.47765900	-1.62623100	2.60660900
C	-1.29390100	-3.19164700	-1.14428500
H	-0.62497000	-3.59864000	-0.38700000
H	-2.06349400	-3.92425100	-1.39279700
H	-0.70193900	-2.98244400	-2.04539600
C	-2.96002400	-1.47982200	-1.50787300
H	-2.54488300	-1.20239700	-2.48656600
H	-3.72175400	-2.24594800	-1.66020600
H	-3.43460900	-0.60296500	-1.07378900

Allene 15 M052X/6-31G*

0 1

C	1.59569300	0.08307800	-0.30068600
C	1.19558600	-1.25805200	0.11923900
C	-0.02300900	-1.78632900	-0.13612600
C	0.71962500	1.14369000	-0.30903300
C	-1.23814200	-1.23909100	-0.36758000
C	-0.70637000	1.15717600	0.00008800
C	-1.59201000	0.09983800	0.09255200
C	2.37046600	-1.89001700	0.68131600
H	2.35529800	-2.87520800	1.12105300
C	3.47255400	-1.12267100	0.44252000
C	3.06784700	0.11109700	-0.27837600
C	-3.05619500	0.13837000	0.19001700
C	-2.45272600	-1.83329000	-0.88877000
C	-3.52493000	-1.05681800	-0.55601100
C	-1.10564400	2.57343200	0.06459000
H	-2.11773800	2.89973000	0.23957600
C	-0.07269600	3.38108800	-0.19232700
H	-0.10876700	4.46068300	-0.23343400
C	1.16203000	2.58554800	-0.48486700
H	2.00144400	2.83573100	0.17199000
H	1.49297500	2.77830600	-1.51165800
C	3.85989100	1.05832100	-0.85209900
H	3.35866900	1.82996000	-1.42206100
C	5.28213400	1.16966000	-0.83566000
C	6.22264500	0.35896300	-0.24131100
C	4.82758400	-1.47516000	0.80922000
C	6.00715900	-0.83725800	0.51557600
H	-2.48588600	-2.80493400	-1.35707400
C	-4.90640100	-1.36549300	-0.85316900
C	-6.05257300	-0.74943100	-0.41435300
C	-3.78616300	1.02349300	0.92429800
H	-3.22354500	1.73378500	1.51998200
C	-5.20208600	1.12331700	1.05386900
C	-6.19499900	0.36600100	0.47154700
C	-5.28994500	-2.47608400	-1.73672400
H	-4.58050100	-3.12101300	-2.23377100
C	-6.62589500	-2.54376400	-1.83601300
H	-7.19162700	-3.25417300	-2.42105600
C	-7.49368400	0.89038800	0.91618400
H	-8.44635000	0.48142700	0.60905800
C	-7.31136800	1.92915400	1.74712400
H	-8.08502900	2.50797200	2.23019300
C	5.13813200	-2.66658300	1.61314600
H	4.39205300	-3.34863800	1.99291300
C	6.46255400	-2.76034100	1.80351100
H	6.97866900	-3.53037600	2.35827200
C	7.55291100	0.92262400	-0.50990300
H	8.47634600	0.48418500	-0.15761100

C	7.43972800	2.03903300	-1.24710200
H	8.24969200	2.66239800	-1.59670400
C	7.14796500	-1.61461400	1.12581300
H	7.85569900	-1.95806100	0.36217800
H	7.72045700	-1.00450300	1.83430700
C	5.99273500	2.30630700	-1.52855200
H	5.67362700	3.28000900	-1.13867300
H	5.78185200	2.31541400	-2.60449800
C	-5.84445200	2.17925400	1.91957300
H	-5.53425600	2.08208800	2.96676800
H	-5.56157900	3.18970500	1.60204100
C	-7.24501200	-1.46227700	-1.00494200
H	-7.89565900	-1.87322100	-0.22406600
H	-7.86348600	-0.78660400	-1.60718300

Allene 16 M052X/6-31G*

0 1

C	-1.58773600	0.25742500	0.34552600
C	-1.26976700	-1.13901300	-0.09389000
C	0.00964700	-1.46709400	-0.08934500
C	-0.65579100	1.33234600	0.17355400
C	1.28570800	-1.12392300	-0.05417000
C	0.66168800	1.35029000	-0.27874300
C	1.61743000	0.28144300	-0.43359700
C	-2.50308900	-1.83910400	-0.42053300
H	-2.56098200	-2.86756800	-0.74063000
C	-3.50667200	-0.98865100	-0.05916900
C	-2.97152600	0.30175100	0.36494600
C	3.00033600	0.33070600	-0.38577800
C	2.50684300	-1.84108100	0.28667600
H	2.55088700	-2.88111600	0.57011800
C	3.52229900	-0.98021200	-0.00072900
C	1.05255200	2.75733800	-0.46404900
H	2.02118400	3.05879100	-0.83378400
C	0.04912000	3.57701400	-0.12510500
H	0.06047100	4.65669400	-0.15625800
C	-1.12991100	2.76150900	0.31069000
H	-2.00533900	2.94740400	-0.32156000
H	-1.42941100	2.98354500	1.34145700
C	-4.08285300	1.19258900	0.53372800
H	-4.03660600	2.22789700	0.83848300
C	4.12092900	1.22617900	-0.44913400
H	4.09646200	2.27976900	-0.68315900
C	5.28137900	0.52863600	-0.20601400
C	4.97571500	-0.89626900	0.07241800
C	-4.96233900	-0.89987900	-0.06427600
C	-5.25507300	0.50821700	0.30676800
C	5.81302700	-1.92431400	0.34788300
H	5.34520500	-2.88950600	0.51183000
C	6.59456400	1.11018800	-0.22648600
H	6.61188700	2.17311900	-0.44601300

C	-5.81279300	-1.91176400	-0.35901500
H	-5.35403400	-2.86601300	-0.59652900
C	-6.56555200	1.08301400	0.42593300
H	-6.57215900	2.13065600	0.71054800
C	7.24748600	-1.90706600	0.45366900
H	7.70025200	-2.86383300	0.68695300
C	8.09488800	-0.85861000	0.30075500
H	9.14990500	-1.07416800	0.42644500
C	7.79432600	0.51695100	-0.00873200
H	8.66136200	1.16427500	-0.07503900
C	-7.25068000	-1.89017900	-0.40117500
H	-7.71442400	-2.83192600	-0.67098400
C	-8.08906900	-0.85393800	-0.14860900
H	-9.14881600	-1.06362300	-0.24063200
C	-7.77477600	0.50130400	0.22971300
H	-8.63771500	1.14078700	0.37649600

Allene 17 M052X/6-31G*

0 1

C	1.58289900	-0.71734900	0.35366800
C	1.27003500	0.67794400	-0.08036600
C	-0.00785100	1.01665000	-0.08952100
C	0.65414500	-1.79068300	0.15937600
C	-1.28244100	0.66184300	-0.07364200
C	-0.65644900	-1.80492200	-0.31448500
C	-1.60921000	-0.73463900	-0.47562700
C	2.50921300	1.38261100	-0.38143600
H	2.55968800	2.41500900	-0.68567100
C	3.51264300	0.53182300	-0.01123200
C	2.96676000	-0.76278900	0.39947400
C	-2.99376000	-0.78418100	-0.46033500
C	-2.51021900	1.37775800	0.25247800
H	-2.54681900	2.41588500	0.53923700
C	-3.52614900	0.52348100	-0.06313700
C	-1.04371500	-3.21070100	-0.51587700
H	-2.00721000	-3.50926600	-0.90109300
C	-0.04565100	-4.03324200	-0.16763200
H	-0.05689500	-5.11273800	-0.20669300
C	1.12603400	-3.22093000	0.29350800
H	2.01300100	-3.40136400	-0.32421400
H	1.40802000	-3.45053900	1.32762700
C	4.06829000	-1.65403000	0.59449700
H	4.01348500	-2.68880500	0.89921300
C	-4.10718200	-1.67653700	-0.57567200
H	-4.07629700	-2.72389600	-0.83525700
C	-5.27702900	-0.98260300	-0.35140800
C	-4.98062900	0.43203300	-0.02876200
C	4.96736800	0.43568200	0.01603500
C	5.24898500	-0.96912100	0.39704500
C	-5.83629900	1.44362600	0.25724900
C	-6.58246800	-1.57123100	-0.42684100

H	-6.58619600	-2.63061200	-0.67067100
C	5.83599300	1.43728900	-0.26654400
C	6.54939500	-1.55323100	0.54914100
H	6.54184700	-2.60347000	0.83008600
C	-7.28963400	1.43646500	0.30889100
C	-8.13481000	0.38307200	0.09454200
C	-7.79220100	-0.99313200	-0.23692300
C	7.29031300	1.42818200	-0.25857400
C	8.12406200	0.38255300	0.02630500
C	7.76694500	-0.98177600	0.39060800
C	-9.59718100	0.44956800	0.16695200
H	-10.14670100	1.35140200	0.39418400
C	-10.14439200	-0.74743900	-0.08306100
H	-11.20337500	-0.96449600	-0.08981500
C	7.72228000	2.78231100	-0.61880800
H	8.75691800	3.08457100	-0.69080400
C	6.66717600	3.57661200	-0.84215300
H	6.71321700	4.61937900	-1.12325600
C	9.58823600	0.44734700	0.01281400
H	10.14763400	1.34099700	-0.22261000
C	10.12351100	-0.73976300	0.32784000
H	11.18111200	-0.95556400	0.38713600
C	-9.08813500	-1.77888700	-0.35922700
H	-9.19814100	-2.22043300	-1.35515400
H	-9.12664100	-2.60463300	0.35910700
C	9.05592200	-1.76180400	0.59504700
H	9.12462100	-2.61204900	-0.09183800
H	9.12413300	-2.16843700	1.60951300
C	5.37726700	2.82684700	-0.65783300
H	4.73937300	3.26889200	0.11634500
H	4.78168200	2.80095800	-1.57770600
C	-5.36178500	2.84417700	0.58540400
H	-4.73252900	2.84714200	1.48286200
H	-4.75330400	3.26006300	-0.22598100
C	-7.70655200	2.80244700	0.64115000
H	-8.73737000	3.10833500	0.74462700
C	-6.64306300	3.60201900	0.79502900
H	-6.67726500	4.65357000	1.04308900

Allene 18 M052X/6-31G*

0 1			
C	-1.56951500	-0.85471200	-0.40631300
C	-1.26632700	0.52684500	0.08824900
C	0.01034600	0.87026900	0.12403000
C	-0.64306200	-1.92756000	-0.23701200
C	1.28286200	0.50052200	0.11430800
C	0.65823400	-1.96899700	0.26810500
C	1.60349700	-0.90305600	0.47621400
C	-2.51423100	1.21073000	0.39978900
H	-2.57410100	2.23028200	0.74287300
C	-3.50856000	0.37206600	-0.02612700

C	-2.95320000	-0.89942100	-0.48998000
C	2.99106500	-0.95799800	0.47500000
C	2.51811300	1.22433600	-0.17324000
H	2.55697100	2.27192700	-0.42465200
C	3.53164900	0.36197300	0.12689700
C	1.03640300	-3.36820900	0.47348100
H	1.98342400	-3.67029900	0.88960900
C	0.03099700	-4.18615200	0.08007900
C	-1.13008400	-3.35035500	-0.39205400
H	-2.02703800	-3.51465800	0.21549100
H	-1.39282600	-3.58326600	-1.42976100
C	-4.04951000	-1.77895800	-0.75840300
H	-3.98649600	-2.79530600	-1.11983300
C	4.09675800	-1.85610600	0.56780800
H	4.05933000	-2.91221800	0.78785100
C	5.27460800	-1.15670200	0.37656300
C	4.98664500	0.26449800	0.10194000
C	-4.96292100	0.27332000	-0.08828100
C	-5.23636300	-1.10583800	-0.55112700
C	5.85157500	1.27977800	-0.14633100
C	6.57792000	-1.74354400	0.44266100
H	6.58536600	-2.80961600	0.65586900
C	-5.83990500	1.25610400	0.23352600
C	-6.53630200	-1.66963200	-0.76380800
H	-6.53174000	-2.70241600	-1.10457600
C	7.30054200	1.28884600	-0.20092500
C	8.14784200	0.22278800	-0.01644900
C	7.78691300	-1.15361600	0.27407300
C	-7.29178400	1.26970900	0.20080900
C	-8.12551700	0.24295400	-0.16383700
C	-7.75142900	-1.09515700	-0.59990900
C	9.60023100	0.29071900	-0.07931800
H	10.14679000	1.20033300	-0.27058600
C	10.15095900	-0.93231900	0.12949100
C	-7.72148300	2.59744200	0.61999100
H	-8.75455400	2.90200400	0.67603500
C	-6.65253200	3.37584600	0.92362000
C	-9.57914400	0.31199900	-0.17146800
H	-10.13595100	1.18876500	0.11908500
C	-10.11815500	-0.86148400	-0.58931500
C	9.07274200	-1.95394100	0.39212600
H	9.16509700	-2.39840500	1.38822900
H	9.11221400	-2.77115100	-0.33528000
C	-9.03089700	-1.86688500	-0.87633200
H	-9.10779000	-2.74547900	-0.22725900
H	-9.07999500	-2.22104600	-1.91126000
C	-5.36854400	2.61488000	0.70193300
H	-4.72357400	3.08091100	-0.05178000
H	-4.78047600	2.53854700	1.62373300
C	5.36337600	2.68123700	-0.43871200
H	4.74429700	2.69020100	-1.34277000
H	4.74678000	3.07286900	0.37812600

C	7.71684400	2.65178600	-0.49884900
H	8.74640700	2.95317200	-0.60731000
C	6.63821900	3.46810200	-0.61722100
N	0.01698100	-5.56435300	0.01993200
C	1.14199700	-6.22630900	0.64456000
H	2.06716100	-5.86145200	0.19700900
H	1.18406300	-6.04440300	1.72764800
H	1.07104200	-7.29912300	0.46628200
C	-1.26197200	-6.22713600	0.19867600
H	-1.63599300	-6.15726100	1.22947700
H	-2.00239400	-5.79015100	-0.46958300
H	-1.15304400	-7.28038500	-0.06141600
N	-11.44269300	-1.15414600	-0.80667800
N	-6.65052500	4.65309600	1.43142200
N	6.62182600	4.82588600	-0.81349300
N	11.47596400	-1.28542400	0.06447900
C	7.89716100	5.44904200	-1.09749800
H	7.76632100	6.52989800	-1.13447700
H	8.60060200	5.21349700	-0.29817600
H	8.32299800	5.10715800	-2.05027900
C	5.47482900	5.41900200	-1.47789200
H	4.55333400	5.03005500	-1.04906300
H	5.49218800	6.49678500	-1.31612900
H	5.46793800	5.22763800	-2.55895600
C	-12.39854200	-0.15527900	-0.37693300
H	-12.16265400	0.79841100	-0.84999100
H	-13.39686200	-0.45800100	-0.69073000
H	-12.39249400	-0.01599600	0.71253400
C	-11.87874000	-2.53180000	-0.66475300
H	-12.86984600	-2.63499600	-1.10654400
H	-11.20197100	-3.19455400	-1.20076900
H	-11.92903700	-2.85351300	0.38404200
C	-5.51620900	5.51059600	1.13710200
H	-5.54968400	6.37744100	1.79711600
H	-4.58648400	4.97842400	1.32969000
H	-5.51062400	5.86314100	0.09708400
C	-7.93372100	5.32041700	1.48516700
H	-8.63334600	4.71253000	2.05991300
H	-7.81712800	6.27997700	1.98771900
H	-8.35709000	5.48901000	0.48569500
C	12.42341100	-0.19944900	-0.07496800
H	12.16850700	0.39173500	-0.95494400
H	12.42875800	0.46223300	0.80146800
H	13.42169100	-0.61250700	-0.21418100
C	11.93408300	-2.41406200	0.85505300
H	12.00557700	-2.17870700	1.92519500
H	11.25907700	-3.25826900	0.72767800
H	12.91935600	-2.71596000	0.50004000

Allene 19 M052X/6-31G*

0 1

C	-1.58590600	0.83952300	0.69708300
C	-1.22483200	-0.52324900	0.26168500
C	0.04268500	-0.93370500	0.32017300
C	-0.75433500	1.90317900	0.52250600
C	1.27330500	-0.41891500	0.37523700
C	0.63007000	1.95202200	0.03392800
C	1.54299400	0.94147300	-0.12097200
C	-2.46463900	-1.21750000	-0.11357900
H	-2.47729100	-2.20881600	-0.54190000
C	-3.51867700	-0.45184500	0.26932000
C	-3.03572800	0.82913600	0.82161000
C	2.99093500	1.01491700	-0.26268200
C	2.55483700	-1.01863900	0.77417100
H	2.62996500	-1.99002900	1.23973600
C	3.55550900	-0.20860900	0.34567100
C	0.94491400	3.37101800	-0.16778500
H	1.89965200	3.71224600	-0.53928900
C	-0.08349800	4.15051200	0.18748900
H	-0.09937500	5.23047900	0.14290500
C	-1.23975200	3.32879900	0.68212800
H	-2.15868400	3.49990000	0.10922400
H	-1.47540000	3.55204900	1.72860100
C	-4.11465700	1.58367200	1.13797100
H	-4.13504000	2.57362200	1.57173300
C	4.02474600	1.80352500	-0.64190600
H	3.99167200	2.76659900	-1.13124000
C	5.28209500	1.11586500	-0.31107800
C	5.00576900	-0.10957800	0.28581900
C	-4.97351600	-0.42288100	0.28887500
C	-5.32683000	0.81269400	0.82118400
C	5.94514400	-1.03884100	0.84009800
C	6.55785100	1.70540100	-0.60035100
H	6.52305300	2.70727400	-1.01770300
C	-5.84945200	-1.49743200	-0.07442300
C	-6.63821000	1.33733300	1.07614500
H	-6.66405900	2.30432700	1.56954000
C	7.31368500	-1.06720300	0.73353200
C	8.17794200	-0.19209500	-0.05368900
C	7.78470000	1.13964500	-0.48602700
C	-7.21786200	-1.51074000	-0.18564800
C	-8.14973300	-0.39627700	-0.03480100
C	-7.83339600	0.81299700	0.70949800
C	9.48585500	-0.44133600	-0.42788400
C	10.10134500	0.76805900	-0.96050000
C	-7.64103100	-2.90293300	-0.41581100
H	-8.67266600	-3.21766000	-0.46919000
C	-6.57018700	-3.70698600	-0.50151200
H	-6.57761800	-4.77469400	-0.66356500
C	-9.45829900	-0.34643800	-0.47948800
C	-10.14763300	0.80134800	0.09799000
C	9.03852400	1.84527500	-0.95045000
H	8.90762900	2.30380300	-1.93276600

H	9.31374900	2.64100800	-0.25087000
C	-9.13505900	1.54619600	0.94060000
H	-9.06480800	2.60043500	0.66490400
H	-9.41805200	1.50135400	1.99715600
C	-5.32764800	-2.89206800	-0.31730000
H	-4.72029100	-3.24427400	0.52340000
H	-4.68789500	-2.92221300	-1.20737200
C	5.50551500	-2.14952800	1.76182500
H	4.90489400	-1.76509500	2.59319900
H	4.88196000	-2.87679100	1.22784200
C	7.81692800	-2.12013600	1.63232800
H	8.86525300	-2.31339600	1.80464300
C	6.79428500	-2.75594600	2.22421400
H	6.86386800	-3.56692800	2.93399000
C	10.11989200	-1.74871600	-0.43923400
H	9.45046700	-2.58045300	-0.25621500
C	-10.03372200	-1.21488500	-1.49241400
H	-9.32154400	-1.84942200	-2.00566700
C	-11.30997000	-1.28916200	-1.92625000
H	-11.49531100	-2.00301900	-2.72160100
C	-12.48172000	-0.54450200	-1.50074300
H	-13.41910900	-0.87611200	-1.93233300
C	11.40179300	-2.07171500	-0.71245300
H	11.63531600	-3.13068100	-0.68698500
C	12.52450600	-1.21575800	-1.05172600
H	13.48357400	-1.71721900	-1.11178400
C	11.37224900	1.00697000	-1.35004900
H	11.59107000	2.01674900	-1.68244900
C	12.50368900	0.10240200	-1.33922000
H	13.45191700	0.55763000	-1.60385800
C	-11.44186800	1.17845200	0.01817500
H	-11.71815700	2.06779800	0.57556800
C	-12.53048800	0.52353100	-0.67768500
H	-13.50743300	0.96358200	-0.50922600

PROTONATED

Allene 1H M052X/6-31G*

1 1			
C	-1.44769700	-0.69717400	0.00000000
C	-1.44769700	0.69717400	0.00000000
C	-0.35756400	1.56666700	0.00000000
C	-0.35756400	-1.56666700	0.00000000
C	1.00186200	1.25633000	0.00000000
C	1.00186200	-1.25633000	0.00000000
C	1.60681000	0.00000000	0.00000000
H	-2.42404900	-1.16733200	0.00000000
H	-2.42404900	1.16733200	0.00000000
H	-0.59873000	2.62307200	0.00000000

H	-0.59873000	-2.62307200	0.00000000
H	1.67751800	2.10342900	0.00000000
H	1.67751900	-2.10342900	0.00000000
H	2.69046100	0.00000000	0.00000000

Allene 2H M052X/6-31G*

1	1		
C	0.50095200	-0.69260600	0.00000100
C	0.49479700	0.73006800	0.00000700
C	-0.61294200	1.58908200	0.00006300
C	-0.56561700	-1.56937400	0.00003000
C	-1.95508200	1.24867900	0.00002300
C	-1.93483500	-1.26714300	-0.00001800
C	-2.54658600	-0.02344100	-0.00004400
H	-0.38766800	2.64948000	0.00011400
H	-0.31535300	-2.62494600	0.00008300
H	-2.64796800	2.08165500	0.00004100
H	-2.60096200	-2.12136700	-0.00003700
H	-3.62984000	-0.03211400	-0.00010100
C	1.87004600	1.19292800	-0.00003200
H	2.15311500	2.23543800	-0.00003500
C	2.70255600	0.13306700	-0.00006400
H	3.78215900	0.17740400	-0.00010400
C	1.93495900	-1.14733700	0.00002400
H	2.15852300	-1.76450800	0.87804300
H	2.15849900	-1.76458100	-0.87794800

Allene 3H M052X/6-31G*

1	1		
C	0.66340500	-0.14191100	-0.00003200
C	1.39472500	1.07948700	-0.00002200
C	2.78341900	1.26395900	0.00002000
C	1.15379300	-1.43341100	-0.00001000
C	2.48841200	-1.86186100	0.00000700
C	3.64599500	-1.09909400	0.00002200
H	3.12084900	2.29436600	0.00003600
H	0.41184000	-2.22466600	-0.00001200
H	2.63261000	-2.93565800	0.00000900
H	4.57645400	-1.65378700	0.00003000
C	0.44338500	2.17269100	-0.00006400
H	0.72590800	3.21562800	-0.00006900
C	-0.80760100	1.67365800	-0.00009900
H	-1.71038900	2.26769200	-0.00014500
C	-0.81598000	0.17280400	-0.00005600
C	-1.51396800	-0.39312600	1.26961400
H	-1.04020100	0.02371000	2.16090300
H	-1.35918200	-1.47631700	1.28914500
C	-1.51403900	-0.39325900	-1.26960600
H	-1.04033200	0.02347600	-2.16097500
H	-1.35926000	-1.47645400	-1.28903600

C	-3.01803500	-0.11085600	1.26051600
H	-3.46104600	-0.55652800	2.15274900
H	-3.19899800	0.96620200	1.32854500
C	-3.01810700	-0.11098800	-1.26045000
H	-3.46117000	-0.55674800	-2.15261200
H	-3.19907000	0.96606400	-1.32857800
C	-3.67739700	-0.67142100	0.00008000
H	-3.58461800	-1.76300200	0.00013500
H	-4.74402100	-0.44323500	0.00009900
C	3.77504300	0.29659100	0.00003400
H	4.79232100	0.66967100	0.00005500

Allene 4H M052X/6-31G*

1 1

C	-0.50096500	-0.69261900	0.00000000
C	-0.49479100	0.73005600	-0.00000100
C	0.61294800	1.58907500	-0.00000100
C	0.56561700	-1.56937200	0.00000000
C	1.95508400	1.24868200	-0.00000100
C	1.93483300	-1.26714300	-0.00000100
C	2.54658300	-0.02344500	-0.00000100
H	2.64797800	2.08165000	-0.00000200
H	3.62983700	-0.03211600	-0.00000200
C	-1.87003100	1.19293300	0.00000200
H	-2.15310000	2.23544300	0.00000500
C	-2.70255200	0.13308100	-0.00000400
H	-3.78215500	0.17741300	-0.00000400
C	-1.93496800	-1.14732600	0.00000400
H	-2.15853600	-1.76454500	-0.87798000
H	-2.15853500	-1.76453600	0.87799600
H	0.38765300	2.64946900	0.00000000
H	0.31535300	-2.62494500	0.00000100
H	2.60096000	-2.12136700	-0.00000100

Allene 5H M052X/6-31G*

1 1

C	-0.66345500	-0.14200800	-0.00004400
C	-1.39462000	1.07942700	-0.00003000
C	-2.78325600	1.26405000	0.00002900
C	-1.15389700	-1.43345800	-0.00002100
C	-3.77494600	0.29678000	0.00005200
C	-2.48851200	-1.86175900	0.00000000
C	-3.64599900	-1.09886700	0.00003000
H	-0.41197100	-2.22472500	-0.00002700
H	-4.79218000	0.66993200	0.00008800
H	-2.63287600	-2.93551800	-0.00000400
H	-4.57647900	-1.65349500	0.00004400
C	-0.44321000	2.17255100	-0.00008800
H	-0.72574000	3.21547300	-0.00009500
C	0.80769100	1.67342700	-0.00012700

H	1.71054900	2.26731600	-0.00018500
C	0.81598700	0.17255500	-0.00007000
C	1.51399600	-0.39337600	-1.26962100
H	1.04026700	0.02336200	-2.16099300
H	1.35939900	-1.47657300	-1.28919600
C	1.51390200	-0.39321000	1.26963100
H	1.04009700	0.02365200	2.16090400
H	1.35929400	-1.47640300	1.28933200
C	3.01799200	-0.11098400	-1.26044200
H	3.19874800	0.96607200	-1.32864000
H	3.46109800	-0.55676700	-2.15257200
C	3.67739600	-0.67117300	0.00010500
C	3.01789700	-0.11082400	1.26053200
H	3.19865300	0.96623900	1.32861000
H	3.46093500	-0.55650000	2.15275000
H	4.74392700	-0.44256600	0.00013100
H	3.58507400	-1.76276800	0.00017100
H	-3.12058700	2.29447600	0.00004900

Allene 6H M052X/6-31G*

1	1		
C	0.67551500	-0.56832000	-0.00001500
C	1.56277600	0.55035000	0.00004500
C	1.27346400	1.89600100	0.00007100
C	-0.71420100	-0.54435000	-0.00001700
C	0.01270500	2.52035100	0.00003400
C	-1.57335900	0.57771400	-0.00001000
C	-1.24140200	1.94494400	-0.00000500
H	2.12691700	2.56535900	0.00011300
H	-2.08192200	2.62932400	-0.00002300
C	2.97443600	0.02144300	0.00008400
H	3.53111400	0.36689500	0.87835100
C	2.78648300	-1.46074700	-0.00003200
H	3.60784700	-2.16274700	-0.00006200
C	1.48032500	-1.78253800	-0.00010300
H	1.07186100	-2.78184100	-0.00018100
C	-1.56646100	-1.78498800	-0.00004000
H	-1.36903200	-2.40916200	-0.87929500
H	-1.36900800	-2.40934000	0.87907400
C	-2.94883500	0.10007400	0.00002900
H	-3.80907100	0.75338700	0.00007400
C	-2.96033800	-1.24493200	-0.00005400
H	-3.83962900	-1.87248500	-0.00005100
H	0.03298100	3.60348800	0.00004500
H	3.53129600	0.36710400	-0.87797700

Allene 7H M052X/6-31G*

1	1		
C	-1.19547300	0.76961800	-0.00002500
C	-1.46906800	2.16197300	-0.00015800

C	-0.59347500	3.26079600	-0.00026300
C	0.06306800	0.16434900	0.00002700
C	0.78439900	3.25712300	-0.00029000
C	1.34277800	0.81078300	-0.00006700
C	1.65052700	2.15309900	-0.00021300
H	-1.07169500	4.23374200	-0.00033900
H	2.70724800	2.39591400	-0.00027200
C	-2.90927600	2.34879900	-0.00017000
H	-3.38537800	3.31880400	-0.00026100
C	-3.51443100	1.15105700	-0.00005300
H	-4.58286500	0.99181400	-0.00003500
C	-2.52320700	0.02259800	0.00005300
C	-2.71494100	-0.82992300	1.28790300
H	-2.67821400	-0.16638500	2.15500200
H	-1.88602900	-1.53169500	1.38982600
C	-2.71495100	-0.83019500	-1.28761200
H	-2.67823200	-0.16684300	-2.15485300
H	-1.88603800	-1.53198700	-1.38939300
C	-4.02600800	-1.61967500	1.25911600
H	-4.07710700	-2.24223200	2.15420700
H	-4.88081200	-0.93846000	1.30547400
C	-4.02601400	-1.61994700	-1.25865100
H	-4.07711500	-2.24269800	-2.15360700
H	-4.88082100	-0.93874400	-1.30515300
C	-4.12409600	-2.48178000	0.00032600
H	-3.31134900	-3.21762900	0.00040500
H	-5.05953000	-3.04308100	0.00038900
C	2.43783300	-0.23878000	-0.00000300
C	0.31820500	-1.27481400	0.00017800
H	-0.44203700	-2.03663100	0.00027500
C	1.64104100	-1.50677100	0.00016800
H	2.09171300	-2.48888500	0.00026500
C	3.32738200	-0.13002100	1.26822900
H	2.70292700	-0.23231500	2.15865000
C	3.32720700	-0.13029400	-1.26839200
H	2.70262200	-0.23278400	-2.15870000
C	4.45315100	-1.16685800	-1.26148900
H	4.03524600	-2.17592300	-1.33024500
H	5.06691200	-1.02417400	-2.15279500
C	4.45332100	-1.16659100	1.26139100
H	5.06720400	-1.02372300	2.15258400
H	4.03542400	-2.17564000	1.33041300
C	5.30878400	-1.04275700	-0.00012000
H	5.80864000	-0.06790400	-0.00025600
H	6.09262600	-1.80163900	-0.00009300
H	3.77166800	0.86976300	1.29234100
H	3.77148000	0.86948900	-1.29277900
H	1.26298600	4.22911200	-0.00038600

Allene 8H M052X/6-31G*

C	-0.71421800	-0.54472300	-0.00001300
C	-1.57318100	0.57746100	-0.00001500
C	-1.24140200	1.94469700	-0.00002800
C	0.67564800	-0.56859000	-0.00000900
C	0.01253800	2.52009800	-0.00003700
C	1.56254600	0.55025300	-0.00000300
C	1.27310700	1.89593700	-0.00002100
H	0.03271600	3.60366400	-0.00005900
H	2.12701200	2.56536300	-0.00002600
C	-2.94862100	0.09999500	0.00001500
H	-3.80933400	0.75286800	0.00003600
C	-2.95993700	-1.24499700	-0.00001400
H	-3.83952500	-1.87256000	-0.00000900
C	-1.56641000	-1.78467000	0.00002200
H	-1.36861900	-2.40847600	-0.87928100
H	-1.36863200	-2.40842100	0.87936900
C	2.97374500	0.02174700	0.00003700
H	3.52994700	0.36759300	-0.87822400
H	3.52991100	0.36758800	0.87832400
C	1.48069900	-1.78256800	0.00003000
H	1.07338400	-2.78241200	0.00004500
C	2.78666300	-1.46003900	0.00001000
H	3.60842700	-2.16194400	0.00002700
H	-2.08235400	2.62914200	-0.00003700

Allene 9H M052X/6-31G*

1 1

C	-1.19547400	0.76962000	-0.00002200
C	-1.46906900	2.16197400	-0.00010300
C	0.06306700	0.16435000	0.00001400
C	0.78439700	3.25712200	-0.00016700
C	1.34277500	0.81078200	-0.00003300
C	1.65052400	2.15309900	-0.00011300
H	1.26298400	4.22911200	-0.00022100
H	2.70724600	2.39591200	-0.00013700
C	-2.90927900	2.34879900	-0.00012000
H	-3.38538000	3.31880400	-0.00017800
C	-3.51443300	1.15105700	-0.00005300
H	-4.58286700	0.99181300	-0.00004900
C	-2.52320600	0.02259800	0.00001900
C	0.31820200	-1.27481400	0.00009900
H	-0.44204300	-2.03662800	0.00015100
C	1.64103600	-1.50677200	0.00010200
H	2.09170900	-2.48888700	0.00015900
C	4.45327300	-1.16664800	1.26143500
H	5.06712400	-1.02381800	2.15265600
H	4.03537700	-2.17570300	1.33039600
C	5.30877900	-1.04275200	-0.00004000
H	6.09262300	-1.80163200	-0.00002100
H	5.80863300	-0.06789700	-0.00011300
C	4.45319000	-1.16679600	-1.26144500

H	5.06698200	-1.02406800	-2.15272300
H	4.03529100	-2.17585900	-1.33026200
C	3.32732900	-0.13008300	1.26828300
H	2.70283800	-0.23242700	2.15867400
H	3.77161000	0.86970200	1.29246500
C	3.32724500	-0.13023400	-1.26833900
H	3.77152000	0.86955100	-1.29266800
H	2.70269100	-0.23268400	-2.15867300
C	2.43783000	-0.23878100	0.00001100
C	-4.02599400	-1.61990200	-1.25876400
H	-4.88080800	-0.93870700	-1.30523700
H	-4.07708500	-2.24261500	-2.15374700
C	-4.02600600	-1.61973500	1.25900300
H	-4.07710900	-2.24233000	2.15406700
H	-4.88082000	-0.93853300	1.30537600
C	-2.71493800	-0.83013600	-1.28768700
H	-1.88601900	-1.53191600	-1.38950400
H	-2.67822500	-0.16673900	-2.15489400
C	-2.71494900	-0.82996900	1.28783500
H	-2.67824200	-0.16645800	2.15495600
H	-1.88603200	-1.53173700	1.38975200
C	-4.12406900	-2.48179000	0.00017600
H	-5.05949500	-3.04310600	0.00020800
H	-3.31131100	-3.21762800	0.00022900
C	-0.59347800	3.26079700	-0.00016200
H	-1.07169700	4.23374300	-0.00021400

Allene 10H M052X/6-31G*

1 1

C	-1.55584600	-0.68156200	0.00000500
C	-1.24903600	0.71383300	0.00004200
C	0.00000000	1.32923500	0.00000000
C	-0.70361500	-1.76167300	-0.00001300
C	1.24903600	0.71383300	-0.00004200
C	0.70361500	-1.76167300	0.00001300
C	1.55584600	-0.68156200	-0.00000500
H	-1.17212200	-2.74003300	0.00001000
H	1.17212200	-2.74003300	-0.00001000
C	-2.50379400	1.45044300	-0.00016100
H	-2.56331600	2.52904800	-0.00030500
C	-3.53781400	0.58977600	0.00001600
H	-4.58410500	0.85956900	-0.00002600
C	-3.05616500	-0.82486300	0.00007900
H	-3.40492000	-1.37938200	0.87845500
H	-3.40504700	-1.37965400	-0.87806600
C	3.05616500	-0.82486300	-0.00007900
H	3.40504600	-1.37965400	0.87806700
H	3.40492000	-1.37938300	-0.87845500
C	2.50379400	1.45044300	0.00016100
H	2.56331600	2.52904800	0.00030500
C	3.53781400	0.58977600	-0.00001600

H	4.58410500	0.85956900	0.00002600
H	0.00000000	2.41404300	0.00000000

Allene 11H M052X/6-31G*

1 1			
C	-1.55996900	0.00686700	0.00003600
C	-1.22012500	-1.38365000	-0.00004900
C	0.03476100	-1.97408700	-0.00008400
C	-0.72349600	1.09249900	0.00002000
C	1.27999000	-1.33932900	-0.00002300
C	0.70772400	1.12142900	-0.00002900
C	1.58134600	0.04733500	-0.00000500
C	-2.46296500	-2.14739500	-0.00002900
H	-2.49738500	-3.22713700	-0.00007500
C	-3.51453500	-1.31285100	0.00002900
H	-4.55475400	-1.60492700	0.00003100
C	-3.06540800	0.11619600	0.00003700
H	-3.43084500	0.65899500	-0.87854700
H	-3.43079700	0.65892100	0.87868800
C	3.08107900	0.19960700	0.00000800
H	3.43091200	0.75213900	-0.87934700
H	3.43095700	0.75233500	0.87921000
C	2.53892700	-2.07520000	0.00004600
H	2.59864400	-3.15385300	0.00006100
C	3.57023800	-1.21392100	0.00006400
H	4.61772000	-1.47847200	0.00012900
C	1.12644400	2.52086800	-0.00002200
H	2.15663900	2.84426600	-0.00002700
C	0.04827600	3.32061000	-0.00007000
H	0.06350000	4.40090500	-0.00012700
C	-1.21688800	2.51937900	0.00004200
H	-1.83551800	2.73265700	-0.87838700
H	-1.83524700	2.73262700	0.87868500
H	0.05377500	-3.05859600	-0.00012100

Allene 12H M052X/6-31G*

1 1			
C	-1.59468300	0.07887000	-0.00002900
C	-1.28021400	-1.29440600	0.00004900
C	-0.04066300	-1.93053600	0.00006400
C	-0.69513600	1.16774000	-0.00002600
C	1.21450600	-1.35109600	0.00000600
C	0.71249800	1.12694900	-0.00002100
C	1.56633700	0.02314600	-0.00003000
C	-2.57064100	-2.07070100	0.00011800
H	-2.64348600	-2.72217700	0.87851600
C	-3.61647400	-1.00573000	-0.00004300
H	-4.67700300	-1.21031200	-0.00008900
C	-3.04819500	0.21311200	-0.00005100
C	3.02345200	0.11589700	-0.00001600

C	2.48622300	-2.16044600	-0.00000700
H	2.54632200	-2.81266600	0.87836200
C	3.55733700	-1.11788700	-0.00006000
H	4.61255700	-1.34947400	-0.00008600
H	2.54630000	-2.81282900	-0.87824600
H	-2.64349200	-2.72270900	-0.87785900
H	-3.57610600	1.15370700	-0.00008700
H	3.57244200	1.04553000	0.00000500
C	-1.11041200	2.56795800	-0.00002600
H	-2.13615400	2.90172200	-0.00001900
C	-0.02633400	3.36182600	-0.00002300
H	-0.03104600	4.44196700	-0.00002200
C	1.22315700	2.54388800	-0.00001000
H	1.84561000	2.74607700	0.87920200
H	1.84567900	2.74611000	-0.87916100
H	-0.06616100	-3.01645800	0.00010300

Allene 13H M052X/6-31G*

1 1

C	-0.66817600	2.49712100	-0.25686300
C	-1.51317500	1.45164800	-0.39661700
C	-1.27671000	0.05865400	-0.06416800
C	0.66814900	2.49713500	0.25687900
C	0.00001700	-0.52959500	0.00001500
C	1.51317100	1.45168100	0.39663500
C	1.27673200	0.05867700	0.06419300
H	-1.06231800	3.46965000	-0.52603000
H	-2.49163400	1.68486800	-0.78951600
H	1.06226800	3.46967300	0.52604900
H	2.49161600	1.68492700	0.78954800
N	-2.36303900	-0.72347900	0.07349800
N	2.36305100	-0.72346700	-0.07350000
C	-3.72048700	-0.17655800	0.00069500
H	-4.00210400	0.06779200	-1.02569500
H	-4.41163400	-0.92413800	0.37594600
H	-3.81174300	0.70948200	0.62759100
C	-2.22315300	-2.15845300	0.30395300
H	-1.76188700	-2.65100800	-0.55543100
H	-1.62406600	-2.34818700	1.19663500
H	-3.20796400	-2.58804100	0.45232500
C	3.72052300	-0.17659000	-0.00077800
H	3.81179200	0.70941300	-0.62772300
H	4.00219200	0.06779500	1.02558900
H	4.41162400	-0.92421800	-0.37602100
C	2.22311000	-2.15844000	-0.30391900
H	1.76188900	-2.65096600	0.55550600
H	1.62395100	-2.34817000	-1.19655500
H	3.20789800	-2.58805900	-0.45235200
H	0.00003400	-1.60387500	0.00000200

Allene 14H M052X/6-31G*

1 1

C	0.66692000	1.67335000	0.15260000
C	1.58314000	0.62535700	0.11201600
C	1.30129600	-0.76292600	-0.05704200
C	-0.74549200	1.64836300	0.01422700
C	0.01102300	-1.34539000	-0.05959500
C	-1.60718800	0.57734600	-0.10340400
C	-1.28166500	-0.82674600	-0.00005800
C	2.96886700	1.23107300	0.04837400
H	3.47665800	0.92638300	-0.87421400
C	2.71598300	2.70166000	0.09829600
H	3.50467500	3.43980600	0.09655000
C	1.40065200	2.94196300	0.17901300
H	0.93109700	3.91190200	0.24165800
C	-1.53788100	2.91745700	-0.17448300
H	-1.50318700	3.54814200	0.72165300
H	-1.14086200	3.51943900	-0.99922000
C	-2.94492500	1.08649600	-0.43137500
H	-3.79658300	0.46274800	-0.65095800
C	-2.91681500	2.42782400	-0.46819100
H	-3.74815100	3.07735800	-0.69877700
H	0.04638500	-2.41952400	0.01863600
H	3.62237500	0.94572100	0.87436800
N	-2.33122000	-1.69527500	0.09947100
N	2.34458100	-1.63805000	-0.19192600
C	-2.16684600	-3.11018200	-0.19583500
H	-1.68541500	-3.65564700	0.62399600
H	-3.15799400	-3.53398200	-0.35094600
H	-1.59358500	-3.24075500	-1.11237300
C	2.15713500	-2.92373500	-0.85071400
H	3.11793800	-3.23120400	-1.26252400
H	1.81517800	-3.70406400	-0.16092700
H	1.45056200	-2.82524200	-1.67245900
C	3.54776800	-1.58254300	0.64060800
H	3.77851000	-2.59940400	0.96046700
H	4.41047900	-1.18825600	0.10154200
H	3.36479800	-0.99445600	1.53577900
C	-3.45035400	-1.43764100	1.01085800
H	-4.40454100	-1.52536500	0.48951000
H	-3.42212400	-2.17835500	1.81449000
H	-3.36946400	-0.45233200	1.45916600

Allene 15H M052X/6-31G*

1 1

C	-1.58224700	-0.11966600	0.22655600
C	-1.24150500	1.29713800	0.19663400
C	0.00372500	1.90922700	0.24542400
C	-0.69744900	-1.16028500	0.50805100
C	1.26827200	1.32823200	0.24116500
C	0.72633000	-1.12226800	0.61530300
C	1.60632000	-0.07653400	0.30714300

C	-2.44122400	2.05078900	0.10655000
H	-2.46658500	3.12859100	0.08323500
C	-3.52005000	1.20069000	0.03160300
C	-3.03286100	-0.18223600	0.07113400
C	3.04504800	-0.15734800	0.14465100
C	2.46974100	2.07964800	0.17332600
C	3.54655400	1.21804200	0.11434500
C	1.16729500	-2.41819900	1.15236800
H	2.17828900	-2.62573500	1.46292500
C	0.12464800	-3.23955000	1.31125900
H	0.15289000	-4.23679200	1.72539300
C	-1.13066800	-2.57644600	0.84390600
H	-1.92417300	-2.60014800	1.59515300
H	-1.50075900	-3.09728900	-0.04618600
C	-3.78379600	-1.32957300	-0.10301700
H	-3.24534900	-2.26363000	-0.13169000
C	-5.16483000	-1.47894900	-0.27706400
C	-6.17261700	-0.51313400	-0.31185200
C	-4.88337400	1.63913400	-0.06608300
C	-6.03934600	0.88963500	-0.20549300
H	2.50423400	3.15707300	0.13768400
C	4.91626300	1.62837200	0.03066200
C	6.05184700	0.85369200	-0.15547000
C	3.74791400	-1.31496700	-0.14691800
H	3.16064700	-2.21886700	-0.25240600
C	5.11508600	-1.48616800	-0.37368000
C	6.14636400	-0.53990800	-0.35845300
C	5.32982900	3.02894000	0.14083300
H	4.65084600	3.85204400	0.30226500
C	6.66538300	3.11835000	0.03159200
H	7.25020100	4.02505000	0.08468100
C	7.40601100	-1.23434300	-0.62436000
H	8.36909900	-0.74685900	-0.66517700
C	7.17402400	-2.54524800	-0.81023900
H	7.91915700	-3.29733700	-1.02575400
C	-5.25931900	3.05482000	-0.02629500
H	-4.55918700	3.86842100	0.08312900
C	-6.59241100	3.17497000	-0.13564200
H	-7.15179600	4.09898800	-0.13223400
C	-7.45394300	-1.19340500	-0.49873600
H	-8.40587100	-0.68629600	-0.55847800
C	-7.25661400	-2.52028900	-0.58486700
H	-8.02285200	-3.26873700	-0.72575100
C	-7.22041000	1.82465000	-0.26281100
H	-7.77325200	1.72200900	-1.20354200
H	-7.93362700	1.62959200	0.54613200
C	-5.80097100	-2.83674400	-0.45850000
H	-5.60368000	-3.49877100	0.39232200
H	-5.42112400	-3.34748900	-1.35087900
C	5.71382300	-2.83845800	-0.67994400
H	5.51586200	-3.56549000	0.11559000
H	5.30379000	-3.26256300	-1.60369000

C	7.25665600	1.76065700	-0.17285400
H	7.97196600	1.50415300	0.61684100
H	7.79811000	1.69571600	-1.12344500
H	-0.01182800	2.99476500	0.23252300

Allene 16H M052X/6-31G*

1 1

C	-1.57147900	0.35326600	-0.00001500
C	-1.24058800	-1.09105300	-0.00002700
C	0.01958500	-1.68348600	-0.00004000
C	-0.73633000	1.41832100	-0.00001100
C	1.25976700	-1.06228800	-0.00003900
C	0.72743900	1.44154500	-0.00001800
C	1.58980200	0.38223900	-0.00002400
C	-2.43979400	-1.82437800	-0.00003000
H	-2.48440100	-2.90533300	-0.00003900
C	-3.52186900	-0.93474700	-0.00002200
C	-3.02951400	0.40789600	-0.00001100
C	3.04450100	0.43726000	-0.00002500
C	2.46724700	-1.79767400	-0.00006000
H	2.51259500	-2.87851200	-0.00007500
C	3.53761400	-0.90943400	-0.00005200
C	1.12097700	2.85010200	-0.00002100
H	2.14412000	3.18787500	-0.00003200
C	0.04270400	3.64550600	-0.00001300
H	0.06218400	4.72610800	-0.00001600
C	-1.22908300	2.84888500	-0.00000200
H	-1.84517000	3.05936900	-0.88075300
H	-1.84515300	3.05936300	0.88076100
C	-4.09340300	1.29678900	0.00001900
H	-4.06942500	2.37525200	0.00003300
C	4.12316500	1.31515900	0.00002500
H	4.11842300	2.39337100	0.00005600
C	5.31514400	0.54719000	0.00002700
C	4.96269900	-0.88130700	-0.00001400
C	-4.94078700	-0.90033400	0.00000200
C	-5.29270100	0.53141900	0.00001400
C	5.80217800	-1.97693700	-0.00002600
H	5.31242900	-2.94518400	-0.00006800
C	-5.79052800	-1.99418900	0.00000300
H	-5.30551600	-2.96484700	-0.00001400
C	-7.18622000	-2.01267100	0.00001700
H	-7.64175000	-2.99519800	0.00001400
C	-8.06811700	-0.93682000	0.00003200
H	-9.11937400	-1.20077500	0.00004100
C	7.20280000	-2.00350800	0.00000700
H	7.65168600	-2.98911300	-0.00000700
C	8.08664800	-0.93561200	0.00005300
H	9.13716600	-1.20223000	0.00007200
C	6.60177600	1.09646000	0.00006600
H	6.64321400	2.18064800	0.00009200

C	7.82268600	0.44220700	0.00007800
H	8.69661100	1.08205700	0.00011200
C	-6.57227600	1.08469400	0.00003000
H	-6.60923900	2.16912200	0.00004100
C	-7.80081500	0.43514100	0.00003800
H	-8.67113400	1.07977600	0.00005200
H	0.03334000	-2.76958900	-0.00005000

Allene 17H M052X/6-31G*

1 1

C	1.57435600	-0.83160200	0.00001300
C	1.24264100	0.61082200	0.00003900
C	-0.01721900	1.20062800	0.00004000
C	0.73724400	-1.89653100	-0.00000200
C	-1.25850500	0.58092200	0.00002100
C	-0.72449000	-1.92016100	-0.00000500
C	-1.58899500	-0.86185300	0.00000200
C	2.44527800	1.34361500	0.00005600
H	2.47905800	2.42419200	0.00008000
C	3.52998600	0.45952800	0.00004600
C	3.03017500	-0.88658700	0.00001500
C	-3.04341000	-0.91716700	-0.00001000
C	-2.46768500	1.31561100	0.00002200
H	-2.50102300	2.39602500	0.00003300
C	-3.54307600	0.43348700	-0.00000500
C	-1.11761600	-3.32994500	-0.00001900
H	-2.14097100	-3.66716200	-0.00002300
C	-0.03962300	-4.12526300	-0.00002600
H	-0.05854500	-5.20591700	-0.00003500
C	1.23131500	-3.32657900	-0.00002800
H	1.84887200	-3.53545600	-0.88036500
H	1.84890300	-3.53548400	0.88028000
C	4.08693800	-1.77781100	-0.00002600
H	4.05883700	-2.85627300	-0.00005500
C	-4.11418900	-1.79644100	-0.00002500
H	-4.10645400	-2.87474100	-0.00003300
C	-5.31416100	-1.03126700	0.00001700
C	-4.97228200	0.39419200	-0.00002600
C	4.95449000	0.41225700	0.00002500
C	5.29358200	-1.01649600	-0.00002300
C	-5.83631900	1.47463800	-0.00004800
C	-6.59058600	-1.60106300	0.00004700
H	-6.61509100	-2.68727300	0.00005900
C	5.82846800	1.48950300	0.00004700
C	6.56430200	-1.59105500	-0.00005800
H	6.58387900	-2.67741600	-0.00008900
C	-7.25366000	1.50001200	-0.00003300
C	-8.13382800	0.41424000	0.00001100
C	-7.81872000	-0.96990000	0.00005000
C	7.24210600	1.50686400	0.00002700
C	8.11879700	0.41389400	-0.00002400

C	7.79838900	-0.96543100	-0.00006000
C	-9.59318300	0.53691600	0.00002400
H	-10.12400400	1.47655900	0.00000500
C	-10.16030400	-0.67969600	0.00006700
H	-11.22152200	-0.88219200	0.00008300
C	7.67367400	2.90998000	0.00006500
H	8.70524700	3.22788800	0.00006000
C	6.60835900	3.72234900	0.00010700
H	6.63142500	4.80215100	0.00014200
C	9.57864300	0.53142900	-0.00005800
H	10.11320000	1.46892700	-0.00004400
C	10.14073200	-0.68775500	-0.00009600
H	11.20098000	-0.89523400	-0.00012500
C	-9.11420800	-1.74906900	0.00008500
H	-9.19136800	-2.39818100	-0.87897000
H	-9.19134800	-2.39811000	0.87919600
C	9.08924800	-1.75128500	-0.00010400
H	9.16344100	-2.40081100	-0.87919800
H	9.16347300	-2.40083600	0.87897000
C	5.34188600	2.91935300	0.00010200
H	4.72424300	3.12277700	0.88133900
H	4.72422100	3.12283300	-0.88110700
C	-5.34237600	2.90239300	-0.00007100
H	-4.72390900	3.10322000	0.88118800
H	-4.72389400	3.10318500	-0.88132600
C	-7.67559300	2.90552000	-0.00007400
H	-8.70508700	3.23005400	-0.00007800
C	-6.60530300	3.71129200	-0.00009700
H	-6.62261100	4.79124500	-0.00012400
H	-0.03160900	2.28708600	0.00005700

Allene 18H M052X/6-31G*

1 1			
C	-1.57283700	-1.00705300	-0.01547800
C	-1.24478800	0.43645300	-0.01730200
C	0.02357100	1.02334600	-0.02066500
C	-0.73429900	-2.06882800	-0.01926600
C	1.25617700	0.40062000	-0.01974200
C	0.72805200	-2.10951100	-0.02269200
C	1.59160900	-1.03618800	-0.01554600
C	-2.44643400	1.16053800	-0.01806700
H	-2.48149200	2.24156400	-0.02079700
C	-3.53569200	0.27402900	-0.01615600
C	-3.03087000	-1.06840000	-0.01472600
C	3.03284100	-1.09210200	-0.00580400
C	2.47506900	1.14166100	-0.01927500
H	2.50400600	2.22241400	-0.02183900
C	3.54114200	0.26232200	-0.01138700
C	1.11852800	-3.49236000	-0.04220200
H	2.14067300	-3.82465000	-0.07758300
C	0.01905100	-4.30978700	-0.03174400

C	-1.24605800	-3.48986900	-0.02652000
H	-1.86100300	-3.69729600	0.85558200
H	-1.86368600	-3.68300300	-0.90994700
C	-4.08670000	-1.96205700	-0.01393500
H	-4.05836200	-3.04101400	-0.01226900
C	4.10833800	-1.97083600	0.01302400
H	4.09850000	-3.04931600	0.02921700
C	5.30944500	-1.20984500	0.01647400
C	4.98018900	0.21113400	0.00003500
C	-4.95974000	0.22058500	-0.01609800
C	-5.29632400	-1.20286900	-0.01429800
C	5.84691200	1.28426800	-0.00507000
C	6.59297000	-1.77432200	0.03420600
H	6.62216700	-2.86072800	0.04860300
C	-5.84222600	1.29493200	-0.01577500
C	-6.57094200	-1.77077300	-0.01119600
H	-6.59583100	-2.85765700	-0.00739700
C	7.26504700	1.33275800	0.00081400
C	8.15199200	0.24246700	0.02132200
C	7.81326100	-1.13981900	0.03548400
C	-7.24981000	1.33480600	-0.01363300
C	-8.13841300	0.23365100	-0.01432900
C	-7.79960500	-1.14204700	-0.01273500
C	9.58854600	0.37031900	0.03969500
H	10.11360300	1.31065000	0.05456900
C	10.17148600	-0.86902000	0.04859800
C	-7.68596000	2.71883300	-0.00285700
H	-8.71675000	3.03100200	0.01567100
C	-6.60212300	3.54622800	-0.01343600
C	-9.57190300	0.36528700	-0.00925000
H	-10.09655300	1.30562100	0.00581600
C	-10.15618200	-0.87610500	-0.01835900
C	9.10363800	-1.93116600	0.06167200
H	9.16310700	-2.55596200	0.95850000
H	9.18354700	-2.59321700	-0.80614900
C	-9.08721300	-1.93636900	-0.00676200
H	-9.15711000	-2.57110500	0.88247400
H	-9.15991800	-2.58847600	-0.88284100
C	-5.34049100	2.71967400	-0.00818400
H	-4.72030900	2.92276200	-0.88663500
H	-4.72878800	2.90644900	0.88014700
C	5.33704300	2.70657000	-0.03147600
H	4.72778800	2.88077200	-0.92405500
H	4.71222100	2.91654800	0.84219000
C	7.68586800	2.71852100	-0.02599400
H	8.71401000	3.03938300	-0.04792400
C	6.59519400	3.53850100	-0.03079700
H	0.03979100	2.11019100	-0.02329900
N	0.00245700	-5.65810100	-0.00153900
C	1.26864200	-6.36031500	-0.09673600
H	1.09989200	-7.42195800	0.07144800
H	1.73296400	-6.22311900	-1.07895000

H	1.95044000	-5.99106700	0.67030900
C	-1.20159900	-6.41038300	-0.30690200
H	-1.16542700	-7.36684500	0.21366700
H	-2.07849400	-5.86977300	0.04130300
H	-1.30514500	-6.59921300	-1.38083000
N	-11.47260600	-1.17019000	-0.06120500
N	-6.57938600	4.90382400	-0.06667500
N	6.56543800	4.89520000	0.00376000
N	11.49028800	-1.16598300	0.01709800
C	-12.41855100	-0.07420800	0.03686800
H	-12.38189000	0.40478000	1.02123800
H	-12.19448300	0.67187100	-0.72650200
H	-13.42308700	-0.45443400	-0.13614400
C	-11.95156100	-2.50453800	0.25422300
H	-11.26863300	-3.25125200	-0.14524900
H	-12.05542900	-2.66064000	1.33361000
H	-12.92309200	-2.65276100	-0.21481000
C	-7.84838300	5.59345900	0.05879400
H	-7.69552100	6.65696200	-0.11453900
H	-8.54155000	5.21763100	-0.69458500
H	-8.29478100	5.45237600	1.05014700
C	-5.39191300	5.62531200	0.35359800
H	-4.50196200	5.14657900	-0.05123000
H	-5.43634500	6.63881100	-0.04267800
H	-5.29915000	5.67941800	1.44495200
C	5.37416000	5.60985500	-0.41762100
H	5.40936500	6.62183100	-0.01639500
H	5.28633900	5.66846600	-1.50898500
H	4.48613700	5.12246700	-0.01934300
C	7.83072900	5.59266100	-0.11785500
H	8.28466100	5.44688900	-1.10489800
H	7.66900600	6.65637400	0.04574000
H	8.52114400	5.22761700	0.64330000
C	11.96395100	-2.48959500	0.38164600
H	11.28806400	-3.24896500	-0.00594600
H	12.94300200	-2.65138300	-0.06705800
H	12.05085800	-2.61352800	1.46696200
C	12.43338700	-0.06835100	0.11625100
H	13.43982800	-0.44765600	-0.04841600
H	12.21304500	0.67289800	-0.65284500
H	12.38999300	0.41699700	1.09761100

Allene 19H M052X/6-31G*

1 1

C	1.56449600	0.93858500	-0.09950800
C	1.22562300	-0.49549400	-0.07754000
C	0.00281100	-1.09468500	-0.01770000
C	0.69880800	2.01722400	-0.05739900
C	-1.27959400	-0.48948700	0.04235300
C	-0.71745900	2.03369300	0.01418800
C	-1.61651100	0.95827900	0.05856900

C	2.47524700	-1.23934700	-0.13701600
H	2.51083300	-2.32012200	-0.13472600
C	3.51687600	-0.36259300	-0.19373100
C	2.98607400	0.99337300	-0.17335300
C	-3.02252200	1.02290900	0.12416400
C	-2.44931900	-1.22698900	0.09737200
H	-2.48816400	-2.30584700	0.09589500
C	-3.54126200	-0.31409900	0.14666900
C	-1.13351300	3.43837700	0.03379600
H	-2.15983600	3.76125700	0.08471300
C	-0.06366300	4.24556400	-0.02039100
H	-0.08562400	5.32600000	-0.01995500
C	1.19803100	3.44131200	-0.08450900
H	1.86043400	3.65351900	0.76229600
H	1.76778600	3.65194700	-0.99664500
C	4.06297800	1.85998400	-0.24003900
H	4.04534100	2.94022600	-0.25796300
C	-4.12869200	1.93518200	0.18530000
H	-4.10082300	3.01311600	0.20402000
C	-5.29137000	1.20539500	0.22775900
C	-4.94136800	-0.26274800	0.20540900
C	4.96090000	-0.28491800	-0.26361600
C	5.27291200	1.09863000	-0.29438300
C	-5.81444400	-1.33795500	0.30303700
C	-6.59208800	1.75898300	0.30680000
H	-6.62355300	2.84358300	0.36314500
C	5.84986000	-1.38016400	-0.36493000
C	6.57253300	1.70470500	-0.39722200
H	6.57026900	2.78644700	-0.48986200
C	-7.22656900	-1.36916500	0.31662300
C	-8.12122600	-0.27814500	0.17077800
C	-7.79706700	1.12453400	0.27978900
C	7.23830900	-1.39645600	-0.34557200
C	8.14801600	-0.29235100	-0.14768200
C	7.78342400	1.10604100	-0.33922900
C	-9.52103200	-0.39799400	-0.08351100
C	-10.15829400	0.87863300	0.07562400
C	7.67224300	-2.76945000	-0.63574700
H	8.70110800	-3.06280300	-0.77350500
C	6.60603400	-3.57571600	-0.76612900
H	6.62827200	-4.63073100	-0.99696400
C	9.50236000	-0.38704300	0.16860000
C	10.14278400	0.90542100	0.00788000
C	-9.08896200	1.90801200	0.31714000
H	-9.23390700	2.39562200	1.28645200
H	-9.12829500	2.68893000	-0.44754300
C	9.07048500	1.89899400	-0.37772700
H	9.04492100	2.75397500	0.30112200
H	9.25649000	2.28524800	-1.38471800
C	5.35026400	-2.78700600	-0.57744400
H	4.68907100	-2.85878600	-1.44755400
H	4.78056300	-3.13916700	0.29078600

C	-5.30229600	-2.75234800	0.44427600
H	-4.75515900	-3.06395200	-0.45275900
H	-4.61267500	-2.84958800	1.28875200
C	-7.62726200	-2.75880600	0.57428000
H	-8.63986700	-3.08057100	0.76029900
C	-6.54763800	-3.55315900	0.64765200
H	-6.55573100	-4.61270000	0.85844900
C	-10.16800300	-1.55293800	-0.61250800
H	-9.51094200	-2.34341400	-0.94706000
C	10.15215200	-1.54449200	0.73973300
H	9.48681600	-2.33678900	1.05793600
C	11.46872500	-1.74835100	0.99061000
H	11.71436200	-2.70226000	1.44386400
C	12.60045200	-0.88595900	0.75991100
H	13.56887500	-1.33129300	0.95304800
C	-11.50571600	-1.78485700	-0.79572500
H	-11.75210100	-2.75440400	-1.21327100
C	-12.62326000	-0.95313000	-0.52029400
H	-13.59445500	-1.40788400	-0.67129500
C	-11.48851600	1.20350000	0.06123500
H	-11.71738600	2.24517300	0.26027900
C	-12.61187900	0.36395500	-0.14793900
H	-13.57713400	0.84184300	-0.03103400
C	11.45078900	1.25090100	0.09735400
H	11.68291600	2.29056000	-0.10913000
C	12.58655200	0.41616100	0.38618200
H	13.54851100	0.90896900	0.30498100
H	-0.00220500	-2.18112700	-0.01549500

M062X

Neutral

Allene 1 M062X/6-31G*

0 1			
C	0.69616300	1.27978000	0.21371900
C	1.60088900	0.26531900	0.18670400
C	1.22076500	-1.03739000	-0.35877200
C	-0.69628400	1.27971800	-0.21373400
C	0.00004100	-1.39328800	-0.00003900
C	-1.60092700	0.26518700	-0.18672400
C	-1.22065400	-1.03745800	0.35883600
H	1.06518100	2.25242900	0.53554300
H	2.62245600	0.45932000	0.51132800
H	1.84606500	-1.57715400	-1.06459700
H	-1.06536900	2.25232700	-0.53560500
H	-2.62249100	0.45906800	-0.51142600
H	-1.84580200	-1.57719800	1.06481400

Allene 2 M062X/6-31G*

0	1			
C		0.36605700	-0.61130500	-0.10342900
C		0.54041600	0.75629200	-0.11309900
C		-0.57057200	1.64798300	-0.42887200
C		-0.82768900	-1.39251400	-0.33439500
C		-1.70941500	1.23164800	0.10034100
C		-2.12388100	-1.05009700	-0.08992100
C		-2.44577900	0.22686300	0.54522700
H		-0.47402200	2.47252000	-1.13052300
H		-0.65002600	-2.40378500	-0.70087500
H		-2.90623300	-1.77643500	-0.30536700
H		-3.14619200	0.29509900	1.37395800
C		1.95770000	1.06679400	0.10597800
H		2.35721800	2.07384600	0.15020500
C		2.65153000	-0.07752300	0.22655900
H		3.71838900	-0.17157700	0.39197200
C		1.72204000	-1.24973600	0.09300400
H		1.74977800	-1.89908900	0.97845700
H		1.98864000	-1.88101500	-0.76618700

Allene 3 M062X/6-31G*

0	1			
C		-0.75893100	-0.03434500	-0.18879100
C		-1.42973900	1.15799000	-0.03019000
C		-2.86514000	1.25231400	-0.27666100
C		-1.27972100	-1.33690000	-0.53493600
C		-3.51614500	0.19489000	0.17827800
C		-2.51417800	-1.85462400	-0.27706300
C		-3.49547700	-1.09087800	0.48979800
H		-3.30294600	2.04448000	-0.87865800
H		-0.56616800	-2.01091600	-1.00924000
H		-2.72732900	-2.87652500	-0.58752800
H		-4.06129800	-1.53923500	1.30262500
C		-0.46490700	2.21456100	0.29073900
H		-0.73586000	3.24875700	0.47228400
C		0.77107100	1.69245000	0.31424400
H		1.68644400	2.23615300	0.51961700
C		0.73179500	0.21566900	-0.00592500
C		1.51853100	-0.08364200	-1.30516200
H		1.13605500	0.55262700	-2.11105700
H		1.32934600	-1.12586200	-1.59724300
C		1.30095300	-0.63951300	1.14980700
H		0.76328900	-0.39601400	2.07286300
H		1.09365600	-1.69573400	0.92793000
C		3.02725600	0.10317100	-1.12567300
H		3.54105400	-0.15246500	-2.05903800
H		3.24909700	1.15974900	-0.92634500
C		2.80926600	-0.45384500	1.32578500
H		3.16807700	-1.10533600	2.13032600
H		3.02234300	0.57668500	1.64001100
C		3.55711300	-0.75480900	0.02499200

H	3.42084100	-1.81583000	-0.22818000
H	4.63291600	-0.59547700	0.15618000

Allene 4 M062X/6-31G*

0	1		
C	-0.53120100	0.64524600	0.27331300
C	-0.44552100	-0.78263900	-0.01812600
C	0.70859900	-1.38498300	0.26558800
C	0.52804000	1.47543000	0.08183700
C	2.00195700	-1.17214800	0.45370000
C	1.86144800	1.12577900	-0.38071500
C	2.54694100	-0.04683500	-0.30535100
H	2.60397800	-1.70054600	1.19082900
H	3.53985100	-0.10011900	-0.75064300
C	-1.77826600	-1.20273300	-0.46984200
H	-2.00870100	-2.18735300	-0.85874100
C	-2.65686000	-0.21691100	-0.23111800
H	-3.72629100	-0.27808500	-0.39951200
C	-1.99697300	1.00730600	0.37736900
H	-2.33340000	1.14982100	1.41424800
H	-2.22451000	1.93202400	-0.16426600
H	0.33473100	2.54544600	0.14471000
H	2.38535200	1.95374100	-0.85655100

Allene 5 M062X/6-31G*

0	1		
C	-0.68376000	-0.17326200	0.03814600
C	-1.39238000	1.06515800	-0.27340000
C	-2.62474100	1.19602600	0.21385800
C	-1.33669700	-1.36410400	0.09212600
C	-3.67243200	0.51867500	0.65725400
C	-2.75546300	-1.61511100	-0.11420900
C	-3.83432900	-0.80503600	0.05596700
H	-0.72875000	-2.26487700	0.15902000
H	-4.30231700	0.84427900	1.48307300
H	-2.97005000	-2.62892500	-0.45006600
H	-4.82270000	-1.19440500	-0.18573200
C	-0.44083500	1.91986300	-0.99239200
H	-0.69714700	2.86317200	-1.46012900
C	0.78738800	1.39133700	-0.88752700
H	1.69037100	1.85298300	-1.27317900
C	0.80957500	0.08387700	-0.09646700
C	1.55102100	-1.04383300	-0.83600900
H	1.10394300	-1.18612100	-1.82632300
H	1.40613600	-1.98004300	-0.27887100
C	1.46463300	0.29991500	1.29096800
H	0.95119400	1.11837400	1.80779200
H	1.30214200	-0.61081300	1.88433900
C	3.05480100	-0.77608300	-0.94487200
H	3.23135100	0.10793000	-1.57209000

H	3.54142100	-1.61697500	-1.45105800
C	3.67830700	-0.55405700	0.43521300
C	2.96637800	0.57303500	1.18633100
H	3.13384100	1.52492500	0.66474800
H	3.39086800	0.68962500	2.18949500
H	4.74760700	-0.33592200	0.34011800
H	3.59329200	-1.48161200	1.01894700

Allene 6 M062X/6-31G*

0 1			
C	-0.70477100	-0.45229600	-0.05527100
C	-1.58281100	0.59041900	0.16603500
C	-1.12644000	1.89867300	0.59667000
C	0.73635300	-0.43905200	0.01596100
C	-0.00559900	2.28270900	-0.00046100
C	1.60271000	0.61580500	-0.17901300
C	1.12130400	1.92840400	-0.59777400
H	-1.60846400	2.43899700	1.40883900
H	1.59092100	2.47805200	-1.41032700
C	-2.99610900	0.08920400	0.04403600
H	-3.56977500	0.26887300	0.96427400
C	-2.81641900	-1.37473700	-0.24288100
H	-3.63663300	-2.06604100	-0.39436500
C	-1.50771400	-1.66782700	-0.29090100
H	-1.07993500	-2.64585000	-0.48467800
C	1.56119400	-1.67854400	0.27258100
H	1.30870100	-2.15589100	1.22910400
H	1.39313400	-2.43615600	-0.50614000
C	2.98264600	0.14113500	-0.02271700
H	3.85498300	0.77781800	-0.11904100
C	2.97617100	-1.17610400	0.24007700
H	3.84145900	-1.80916300	0.39660500
H	-3.53748800	0.60262300	-0.76231600

Allene 7 M062X/6-31G*

0 1			
C	1.20964700	0.84290800	-0.10528800
C	1.51366700	2.18976200	-0.08352400
C	0.51386800	3.22064500	-0.35263900
C	-0.10213900	0.23181800	-0.20780000
C	-0.62507900	2.98175600	0.27223200
C	-1.31843700	0.77230200	0.17516000
C	-1.43849200	2.07434900	0.79747900
H	0.67885300	4.01610100	-1.07528200
H	-2.05911300	2.24309700	1.67562900
C	2.94642600	2.36411300	0.16695500
H	3.43088000	3.33098700	0.24768000
C	3.52633100	1.16100200	0.27462700
H	4.58071700	0.97387000	0.44447600
C	2.51609300	0.06048700	0.03577600

C	2.90799700	-0.64956600	-1.29130900
H	3.02113100	0.11075300	-2.07187100
H	2.09895200	-1.31213000	-1.61186200
C	2.46283400	-0.95083200	1.20093400
H	2.26374500	-0.40739500	2.13144800
H	1.61319900	-1.62810500	1.04189500
C	4.18419700	-1.48397300	-1.14863900
H	4.38498600	-2.00308100	-2.09249700
H	5.04431400	-0.82725100	-0.96440500
C	3.74368200	-1.78027400	1.31555000
H	3.63581300	-2.51067700	2.12504500
H	4.58596800	-1.13135100	1.59040500
C	4.06053200	-2.48966600	-0.00237100
H	3.25195700	-3.19900000	-0.23140100
H	4.98070000	-3.07691800	0.09018000
C	-2.44087100	-0.21806800	-0.02949100
C	-0.38403900	-1.16066800	-0.62941100
H	0.36270600	-1.86921100	-0.96372100
C	-1.69610900	-1.42232100	-0.54284400
H	-2.17005100	-2.36300700	-0.80077700
C	-3.45171600	0.32859200	-1.06598100
H	-2.93142100	0.50453400	-2.01391800
C	-3.17506700	-0.51571400	1.29759800
H	-2.46249900	-0.93124900	2.01871500
C	-4.36873500	-1.45336400	1.10047700
H	-4.01468300	-2.43750100	0.76567600
H	-4.87317400	-1.61258800	2.05997500
C	-4.64602000	-0.60745300	-1.25947700
H	-5.34794900	-0.16573800	-1.97541300
H	-4.30462100	-1.55464900	-1.69861800
C	-5.34895700	-0.88875000	0.07007100
H	-5.77432400	0.04823700	0.45625600
H	-6.18550600	-1.58024700	-0.07856100
H	-3.80797700	1.30448100	-0.70785300
H	-3.54028400	0.43553600	1.71028700

Allene 8 M062X/6-31G*

0 1			
C	-0.80172500	-0.46070200	-0.33880200
C	-1.51068200	0.75025600	0.05509400
C	-0.94396200	1.92657400	-0.22195100
C	0.55784200	-0.53966900	-0.26316500
C	0.22515100	2.50000700	-0.47223000
C	1.51337400	0.50913600	0.13809700
C	1.39641000	1.86123900	0.12303400
H	0.34993900	3.32487900	-1.17261300
H	2.24426800	2.45953800	0.45965200
C	-2.80557600	0.32354300	0.60218400
H	-3.52105000	0.99465600	1.06210800
C	-2.98813600	-0.98090600	0.34854100
H	-3.88597600	-1.54427100	0.57685400

C	-1.79839900	-1.59939600	-0.36194200
H	-2.07407300	-1.92094800	-1.37665400
H	-1.41155600	-2.48331200	0.15874500
C	2.81163100	-0.19215300	0.51524700
H	3.68319800	0.26264400	0.02953500
H	2.98725700	-0.13235000	1.59847700
C	1.32618900	-1.79162400	-0.34303600
H	0.89945800	-2.72769800	-0.68690200
C	2.58181400	-1.61475900	0.08628500
H	3.34495000	-2.38242200	0.14666000

Allene 9 M062X/6-31G*

0 1

C	-1.16293600	0.77271500	-0.10543900
C	-1.31264500	2.11949100	0.43400200
C	-0.46810300	3.07044400	0.02840200
C	0.07122500	0.28475300	-0.44270200
C	0.73514100	3.26876500	-0.48282700
C	1.38870300	0.92896700	-0.24081400
C	1.72553000	2.24040300	-0.16284800
H	0.96484100	4.05045300	-1.20568800
H	2.76485300	2.51177900	0.02255300
C	-2.54719300	2.14183000	1.22235600
H	-2.87464200	2.98934500	1.81305800
C	-3.23426000	1.01656600	0.99029200
H	-4.22102400	0.80412100	1.38749700
C	-2.49043300	0.03391400	0.08965200
C	0.37443300	-1.09483700	-0.86397400
H	-0.36947100	-1.78323300	-1.24632200
C	1.67715800	-1.36547400	-0.73240900
H	2.14385700	-2.31312200	-0.97938000
C	3.93828900	-1.51038600	1.40823900
H	4.22932600	-1.61956100	2.45888700
H	3.51640500	-2.47572700	1.09721200
C	5.16152100	-1.18743900	0.54730900
H	5.90953800	-1.98349400	0.62962700
H	5.63113800	-0.26837100	0.92558400
C	4.76346800	-0.97641400	-0.91503200
H	5.64030200	-0.70449600	-1.51285300
H	4.38675900	-1.92033400	-1.33066900
C	2.87394700	-0.41907700	1.27887100
H	1.98571000	-0.66324900	1.87255400
H	3.27453200	0.52640200	1.67068700
C	3.69858100	0.11668000	-1.04293500
H	4.14012800	1.06369900	-0.70736600
H	3.40013100	0.25613600	-2.08822100
C	2.44774100	-0.18262000	-0.19144000
C	-4.56782600	-0.87755000	-1.09149400
H	-5.25484600	-0.23804300	-0.52144000
H	-5.02777100	-1.03128700	-2.07381800
C	-3.70798900	-2.02366100	0.98647600

H	-3.55680900	-2.99226700	1.47566100
H	-4.36074200	-1.43994800	1.64818600
C	-3.22247900	-0.16826900	-1.25698500
H	-2.57591900	-0.77154700	-1.91035800
H	-3.35033500	0.80493500	-1.74397900
C	-2.35544700	-1.32043600	0.82424700
H	-1.88210100	-1.15242500	1.79830200
H	-1.69388600	-1.98567400	0.26137700
C	-4.39757400	-2.21446500	-0.36706700
H	-5.36805900	-2.70509700	-0.23481900
H	-3.78502600	-2.88239900	-0.98955400

Allene 10 M062X/6-31G*

0 1			
C	-1.55687900	0.60235300	0.32884200
C	-1.23546800	-0.74050500	-0.13934600
C	0.00000100	-1.24993800	0.00000500
C	-0.69017400	1.64586400	0.21524300
C	1.23547300	-0.74050600	0.13934300
C	0.69017100	1.64586600	-0.21523200
C	1.55687700	0.60235700	-0.32883600
H	-1.09906100	2.63759400	0.40589200
H	1.09905400	2.63759700	-0.40588500
C	-2.49980900	-1.32726100	-0.60645000
H	-2.57050800	-2.28696000	-1.10484700
C	-3.52538900	-0.55056800	-0.22466500
H	-4.57547900	-0.77952300	-0.36897300
C	-3.05615400	0.68859100	0.51211300
H	-3.45995700	1.61718200	0.09333600
H	-3.36537100	0.65061900	1.56657200
C	3.05615100	0.68859600	-0.51211700
H	3.36535700	0.65063700	-1.56657900
H	3.45996000	1.61718200	-0.09333300
C	2.49981200	-1.32724400	0.60647200
H	2.57051000	-2.28693300	1.10488800
C	3.52539200	-0.55058100	0.22463000
H	4.57548300	-0.77954500	0.36891800

Allene 11 M062X/6-31G*

0 1			
C	-1.56470400	-0.05378800	0.29435000
C	-1.20769900	-1.39649400	-0.15299500
C	0.03270400	-1.89240600	-0.00864900
C	-0.71074800	0.99846700	0.19635600
C	1.26190200	-1.36447700	0.14208200
C	0.70032500	1.01485800	-0.20748700
C	1.58775100	-0.01974700	-0.30600000
C	-2.45544900	-2.01989500	-0.61938100
H	-2.49701900	-2.99166600	-1.09720300
C	-3.50287500	-1.26205100	-0.26296500

H	-4.54618400	-1.51759000	-0.41112200
C	-3.06950600	0.00875700	0.44026500
H	-3.48370400	0.91009700	-0.02747400
H	-3.40481800	0.01615900	1.48753200
C	3.09284400	0.08597600	-0.42987100
H	3.44703000	0.10619900	-1.47071800
H	3.47410200	0.99337800	0.05325400
C	2.51954100	-1.96019400	0.61763000
H	2.58019200	-2.93225400	1.09282900
C	3.55102600	-1.17515400	0.27357100
H	4.59899700	-1.40552900	0.42993200
C	1.06638100	2.43025100	-0.37752000
H	2.04439000	2.75164500	-0.71823600
C	0.04882600	3.23575100	-0.05177500
H	0.06202300	4.31916100	-0.08540900
C	-1.15233600	2.44087200	0.37716000
H	-2.03948900	2.68082700	-0.22424900
H	-1.42341300	2.64522400	1.42223400

Allene 12 M062X/6-31G*

0	1		
C	1.58724600	0.01558000	-0.31117000
C	1.27281700	-1.32472800	0.14353500
C	0.04296300	-1.84266600	-0.00374100
C	0.68619200	1.05426400	-0.21397600
C	-1.20304100	-1.37071100	-0.14533700
C	-0.70547400	1.02761400	0.21189800
C	-1.56090400	-0.03696400	0.30898100
C	2.56466900	-1.96119000	0.62218800
H	2.68684100	-2.96964100	0.21606200
C	3.60544200	-0.99043400	0.11230100
H	4.67084400	-1.15633500	0.22965200
C	3.04839700	0.10211300	-0.43531400
C	-3.02483500	-0.00010300	0.44227100
C	-2.47553800	-2.04161600	-0.62970600
H	-2.52570800	-2.11836600	-1.72570700
C	-3.54573900	-1.10764700	-0.11005100
H	-4.60552000	-1.31008700	-0.22242300
H	-2.56905000	-3.05750700	-0.23445200
H	2.61646500	-2.04846200	1.71741200
H	3.59140300	0.95239500	-0.83296700
H	-3.59044100	0.82960400	0.85252200
C	1.04370600	2.46978800	-0.38926300
H	2.01859000	2.79844600	-0.73141300
C	0.02286800	3.27003600	-0.05751400
H	0.02761600	4.35330900	-0.09223400
C	-1.16463500	2.46446500	0.38745500
H	-2.06119400	2.68623500	-0.20660800
H	-1.42465300	2.67360700	1.43481700

Allene 13 M062X/6-31G*

0 1

C	0.47868300	2.27155100	0.54350400
C	1.23496600	1.23965400	0.99974400
C	1.20306700	-0.06423800	0.34230500
C	-0.47874500	2.27156500	-0.54343800
C	0.00001700	-0.54705800	-0.00006500
C	-1.23500100	1.23967300	-0.99973300
C	-1.20306800	-0.06424100	-0.34233000
H	0.63961600	3.24233500	1.00905500
H	1.93543100	1.42157900	1.81528400
H	-0.63969300	3.24236400	-1.00895100
H	-1.93544900	1.42161200	-1.81528400
N	2.40668000	-0.75928600	0.17545800
N	-2.40664500	-0.75930400	-0.17541800
C	3.59984400	0.00341100	-0.14790300
H	4.48486500	-0.59416900	0.09071200
H	3.64241700	0.27386000	-1.21565000
H	3.64093400	0.92194600	0.43773000
C	2.31211300	-2.00326200	-0.56060100
H	3.25042200	-2.55439000	-0.44741500
H	1.48575300	-2.59271200	-0.15653500
H	2.12310100	-1.84462500	-1.63416200
C	-3.59987200	0.00333400	0.14782900
H	-3.64094500	0.92187000	-0.43780200
H	-4.48484600	-0.59428300	-0.09087100
H	-3.64255800	0.27377500	1.21557200
C	-2.31204600	-2.00327100	0.56065000
H	-3.25033300	-2.55443400	0.44745300
H	-1.48565500	-2.59268900	0.15660000
H	-2.12305800	-1.84461700	1.63421200

Allene 14 M062X/6-31G*

0 1

C	0.32661300	1.61268700	-0.31657000
C	1.39953100	0.74466200	-0.39808500
C	1.38155600	-0.57385700	0.21050800
C	-0.96175400	1.38099800	0.27694600
C	0.23335600	-1.27024600	0.14404100
C	-1.60958600	0.18659800	0.48955400
C	-1.07998400	-1.06942800	-0.02466300
C	2.58806100	1.49353400	-0.94540400
H	3.41134200	1.48423200	-0.21681800
C	2.05514800	2.87732900	-1.17910600
H	2.64164300	3.68703100	-1.59637700
C	0.76776800	2.93094300	-0.80862100
H	0.12298000	3.80199700	-0.86030500
C	-1.84724800	2.49138400	0.79527600
H	-1.33745800	3.10557200	1.54971900
H	-2.14422400	3.17522100	-0.01279600
C	-2.88427500	0.44122300	1.17379400
H	-3.57290600	-0.34277600	1.46964500

C	-3.03449300	1.76296200	1.35885100
H	-3.87165800	2.25838200	1.83580800
H	2.97707500	1.04513000	-1.86987400
N	2.53924000	-1.00825500	0.91966100
N	-1.95126400	-1.99362300	-0.61330200
C	3.58708200	-1.49509300	0.02855000
H	4.49123600	-1.70081300	0.60992700
H	3.28026800	-2.41971100	-0.49052300
H	3.83052300	-0.74566200	-0.72702200
C	2.22105700	-2.01459500	1.91744300
H	1.80959800	-2.93288900	1.46439400
H	3.13056700	-2.26444300	2.47132700
H	1.47853200	-1.61791000	2.61326800
C	-1.32293900	-3.18813900	-1.14289900
H	-0.63551500	-3.58913900	-0.39459400
H	-2.09879500	-3.92574500	-1.36869100
H	-0.74776300	-2.98983400	-2.06130800
C	-2.99509700	-1.47429600	-1.48348000
H	-2.60211500	-1.19179900	-2.47355100
H	-3.75842500	-2.24542800	-1.62393300
H	-3.46950700	-0.59826100	-1.03960700

Allene 15 M062X/6-31G*

0 1

C	1.59546500	0.08194500	-0.29040300
C	1.19677000	-1.26057600	0.13378500
C	-0.02133900	-1.79138300	-0.12241300
C	0.71915600	1.14262400	-0.29835600
C	-1.23666900	-1.24411200	-0.35753200
C	-0.70859400	1.15537700	0.01140500
C	-1.59326200	0.09675500	0.10140800
C	2.37617700	-1.88892000	0.69325600
H	2.36506900	-2.87600400	1.13744700
C	3.47689800	-1.12132800	0.44856600
C	3.06843600	0.11176100	-0.27302900
C	-3.05859000	0.13534800	0.19536900
C	-2.45191900	-1.83824600	-0.87960400
C	-3.52542100	-1.06173200	-0.55030800
C	-1.10772300	2.57236900	0.07721000
H	-2.12269900	2.89956400	0.25525900
C	-0.07444100	3.38068200	-0.17948900
H	-0.10929200	4.46325600	-0.21922100
C	1.15964500	2.58514500	-0.47489700
H	2.00621700	2.83725400	0.17758700
H	1.49050200	2.77887700	-1.50495800
C	3.85806200	1.05984100	-0.84993300
H	3.35194800	1.83462600	-1.41873500
C	5.28199000	1.17264800	-0.84011000
C	6.22584900	0.36221400	-0.25014800
C	4.83537200	-1.47275400	0.80942500
C	6.01372000	-0.83543100	0.50921100

H	-2.48543900	-2.81276500	-1.34985800
C	-4.90755500	-1.37110500	-0.85078100
C	-6.05518400	-0.75270200	-0.41874400
C	-3.79136600	1.02363500	0.92380200
H	-3.22814500	1.73884100	1.52000900
C	-5.20939300	1.12618000	1.04772500
C	-6.20074100	0.36780700	0.46346100
C	-5.28844100	-2.48512900	-1.73214100
H	-4.57384700	-3.13479500	-2.22308800
C	-6.62430600	-2.55198200	-1.83747200
H	-7.19141700	-3.26517200	-2.42316800
C	-7.50122500	0.89605700	0.90007600
H	-8.45548900	0.48618000	0.58707700
C	-7.32158700	1.93795700	1.72837000
H	-8.09776700	2.52163200	2.20796000
C	5.14953000	-2.66397900	1.61300900
H	4.40153800	-3.34701700	1.99694000
C	6.47516200	-2.75823200	1.79741700
H	6.99665500	-3.53013900	2.35008400
C	7.55498800	0.92663200	-0.52517100
H	8.48240500	0.48685800	-0.17434700
C	7.43811200	2.04348700	-1.26194000
H	8.24725500	2.67025100	-1.61630300
C	7.15688400	-1.61325300	1.11442400
H	7.86365200	-1.95815500	0.34616200
H	7.73820300	-1.00111400	1.81862600
C	5.98954600	2.30937400	-1.53596800
H	5.66949700	3.28577600	-1.14539700
H	5.77125800	2.32077500	-2.61336400
C	-5.85502500	2.18584700	1.90609800
H	-5.54776100	2.09463600	2.95771900
H	-5.56742100	3.19774500	1.58724200
C	-7.24516900	-1.46695500	-1.01251400
H	-7.90347100	-1.87482200	-0.23226900
H	-7.86432800	-0.79150300	-1.61978200

Allene 16 M062X/6-31G*

0 1			
C	-1.58529300	0.24871600	0.35028400
C	-1.27050100	-1.15168600	-0.08644000
C	0.00989800	-1.47917500	-0.09203500
C	-0.65437900	1.32525100	0.17371000
C	1.28713500	-1.13658300	-0.06607500
C	0.66053300	1.34341600	-0.28432600
C	1.61596200	0.27320400	-0.44189500
C	-2.50747000	-1.84873700	-0.40683000
H	-2.56724000	-2.88120600	-0.72393000
C	-3.50876000	-0.99443300	-0.04737500
C	-2.96819700	0.29626500	0.36986200
C	2.99781100	0.32562400	-0.39196700
C	2.51189700	-1.85061000	0.26935300

H	2.55778400	-2.89465400	0.54926400
C	3.52519100	-0.98555400	-0.01440400
C	1.05039200	2.75088600	-0.47233800
H	2.02022200	3.05369100	-0.84833500
C	0.04745500	3.57068500	-0.12993900
H	0.05644900	4.65316300	-0.16160800
C	-1.12919900	2.75389800	0.31068000
H	-2.01046800	2.93886700	-0.31957600
H	-1.42975200	2.97822300	1.34390400
C	-4.07701700	1.19331400	0.53225200
H	-4.02556200	2.23321900	0.83247400
C	4.11543700	1.22756900	-0.44476300
H	4.08536300	2.28606100	-0.67129200
C	5.27865700	0.53506400	-0.20250600
C	4.97900400	-0.89506500	0.06407300
C	-4.96503700	-0.89909100	-0.05556600
C	-5.25215400	0.51375300	0.30746600
C	5.82022200	-1.92186800	0.33465300
H	5.35462200	-2.89367500	0.48837600
C	6.59178100	1.12222400	-0.21176400
H	6.60584900	2.19019700	-0.42387600
C	-5.81961700	-1.90906000	-0.34742000
H	-5.36278300	-2.86984600	-0.57827000
C	-6.56272100	1.09385600	0.42106000
H	-6.56607700	2.14588800	0.70242700
C	7.25549600	-1.89943100	0.44776700
H	7.71270300	-2.85928100	0.67479100
C	8.09878700	-0.84555600	0.30856300
H	9.15736800	-1.05747800	0.43868700
C	7.79317400	0.53260700	0.00846800
H	8.66037500	1.18600300	-0.04690700
C	-7.25866900	-1.88177700	-0.39495700
H	-7.72670300	-2.82577800	-0.66267800
C	-8.09359900	-0.84052100	-0.15031500
H	-9.15719500	-1.04616900	-0.24546500
C	-7.77414200	0.51631300	0.22372700
H	-8.63740900	1.16179700	0.36600100

Allene 17 M062X/6-31G*

0 1			
C	1.58041300	-0.70689400	0.36933400
C	1.27053900	0.69293000	-0.06140900
C	-0.00862300	1.02880700	-0.08095700
C	0.65344400	-1.78193800	0.16852500
C	-1.28414200	0.67490400	-0.07599900
C	-0.65354500	-1.79689200	-0.31373300
C	-1.60634600	-0.72571800	-0.47823400
C	2.51316800	1.39453600	-0.35633400
H	2.56716900	2.43168300	-0.65605000
C	3.51378900	0.53864900	0.01065700
C	2.96355200	-0.75586100	0.41516000

C	-2.99002700	-0.77937300	-0.46558500
C	-2.51662300	1.38633500	0.24315200
H	-2.55792400	2.42857200	0.52723300
C	-3.52845600	0.52712000	-0.07345400
C	-1.03798100	-3.20318100	-0.52032800
H	-2.00174200	-3.50368600	-0.91346500
C	-0.04017200	-4.02531500	-0.16807300
H	-0.04807500	-5.10756100	-0.20886100
C	1.12709800	-3.21135400	0.30177300
H	2.02226100	-3.38840000	-0.31113600
H	1.40719400	-3.44431000	1.33892100
C	4.06360900	-1.65274400	0.60366100
H	4.00453600	-2.69171700	0.90518400
C	-4.10140200	-1.67722800	-0.57912200
H	-4.06498400	-2.72836300	-0.83646400
C	-5.27431400	-0.98798000	-0.35803700
C	-4.98266700	0.42946300	-0.03850000
C	4.96824900	0.43602800	0.03151600
C	5.24662000	-0.97208900	0.40620000
C	-5.83902400	1.44056000	0.24875600
C	-6.58149800	-1.57784200	-0.43151200
H	-6.58456900	-2.64075600	-0.67568800
C	5.83680800	1.43678800	-0.25605100
C	6.54892300	-1.55813600	0.55031800
H	6.54145400	-2.61208900	0.83091800
C	-7.29318700	1.43223400	0.30309300
C	-8.13683000	0.37634100	0.09290000
C	-7.79251500	-1.00148000	-0.23910200
C	7.29204000	1.42505100	-0.25928300
C	8.12539400	0.37625600	0.01709000
C	7.76751100	-0.98923400	0.38389900
C	-9.59948400	0.44010100	0.17130800
H	-10.14965800	1.34452800	0.40275400
C	-10.14608300	-0.75820000	-0.07628000
H	-11.20721900	-0.97961100	-0.07826000
C	7.72299000	2.77995900	-0.62027100
H	8.76118800	3.08063700	-0.69800700
C	6.66675000	3.57660100	-0.83406400
H	6.71053000	4.62281500	-1.11396200
C	9.58999300	0.43676900	-0.01126200
H	10.14967000	1.33217600	-0.25464500
C	10.12553600	-0.75241400	0.29773300
H	11.18563900	-0.97378800	0.34511300
C	-9.08871600	-1.78767800	-0.35623800
H	-9.20274500	-2.23349800	-1.35318300
H	-9.12430000	-2.61709700	0.36280200
C	9.05734700	-1.77097300	0.57620000
H	9.11783400	-2.62601900	-0.11045200
H	9.13529100	-2.18065300	1.59209200
C	5.37754100	2.82722700	-0.64283700
H	4.73864400	3.26956900	0.13523500
H	4.77269900	2.80336400	-1.56091700

C	-5.36494200	2.84138600	0.57576500
H	-4.73295000	2.84564200	1.47555100
H	-4.74971500	3.25692900	-0.23536600
C	-7.70994300	2.79953500	0.63292100
H	-8.74443000	3.10517400	0.73611600
C	-6.64596000	3.60016800	0.78401300
H	-6.67879300	4.65509900	1.03068700

Allene 18 M062X/6-31G*

0 1

C	-1.56743100	-0.83664500	-0.44328000
C	-1.26626000	0.55082800	0.04262900
C	0.01173700	0.88972400	0.09101800
C	-0.64354400	-1.91154600	-0.26324300
C	1.28534200	0.52256700	0.09880700
C	0.65258500	-1.95226000	0.25341000
C	1.59800200	-0.88554500	0.46523000
C	-2.51689300	1.23431800	0.34541800
H	-2.57950400	2.26000500	0.68057800
C	-3.50941400	0.38942600	-0.07254900
C	-2.95059000	-0.88460000	-0.52499800
C	2.98403700	-0.94681200	0.47059500
C	2.52728300	1.23890000	-0.17837600
H	2.57444700	2.29003000	-0.42852400
C	3.53407100	0.37013400	0.12800300
C	1.02749600	-3.35141300	0.46806200
H	1.97145400	-3.65602100	0.89859400
C	0.02472400	-4.16983200	0.06853400
C	-1.13091200	-3.33392900	-0.41672200
H	-2.03618600	-3.49776100	0.18524100
H	-1.39075800	-3.57172700	-1.45754800
C	-4.04572100	-1.77182000	-0.77844500
H	-3.97871800	-2.79471700	-1.13064200
C	4.08575600	-1.85288700	0.56484900
H	4.03931200	-2.91278700	0.78132200
C	5.26816500	-1.16108600	0.38054500
C	4.98877700	0.26394000	0.10855400
C	-4.96379800	0.28301000	-0.12288700
C	-5.23469500	-1.10269900	-0.57062200
C	5.85781900	1.27729500	-0.13431700
C	6.57148400	-1.75320200	0.44865900
H	6.57395600	-2.82320700	0.66001200
C	-5.84108400	1.26479100	0.20293100
C	-6.53620900	-1.67305100	-0.76626200
H	-6.53061100	-2.71152500	-1.10065400
C	7.30843000	1.28066700	-0.18388400
C	8.15049600	0.21017500	-0.00248900
C	7.78387400	-1.16828200	0.28383600
C	-7.29446300	1.27046900	0.18939800
C	-8.12774600	0.23664700	-0.15677700
C	-7.75303200	-1.10376300	-0.59112000

C	9.60362600	0.27218100	-0.06474200
H	10.15583700	1.18274800	-0.25548400
C	10.14976300	-0.95344400	0.14039500
C	-7.72516800	2.59909400	0.60555100
H	-8.76215900	2.90051900	0.67255100
C	-6.65616800	3.38554600	0.88854400
C	-9.58196300	0.29736200	-0.14035100
H	-10.14061300	1.17519000	0.15621000
C	-10.12167000	-0.88162900	-0.54163600
C	9.06778600	-1.97184600	0.39949300
H	9.16129400	-2.42413300	1.39565000
H	9.10640700	-2.79099500	-0.33087100
C	-9.03359900	-1.88139500	-0.84439100
H	-9.09660100	-2.76356400	-0.19310500
H	-9.09873900	-2.24196100	-1.87979700
C	-5.37141600	2.62838700	0.65842300
H	-4.72953100	3.09554200	-0.10253200
H	-4.77165100	2.56142300	1.57784900
C	5.37663400	2.68178300	-0.42374700
H	4.75912000	2.69961400	-1.33327000
H	4.75156200	3.07435000	0.39109200
C	7.73013500	2.64438800	-0.47342500
H	8.76442500	2.94454000	-0.57526000
C	6.65498400	3.46510900	-0.59222000
N	0.00802600	-5.55002900	0.01635000
C	1.12408700	-6.21345100	0.65422200
H	2.05846200	-5.84257300	0.22306000
H	1.15144800	-6.03781000	1.74216500
H	1.05954300	-7.28848100	0.46923900
C	-1.27430000	-6.21212700	0.16424500
H	-1.68094800	-6.13518900	1.18570100
H	-1.99904700	-5.78098600	-0.52991300
H	-1.15813900	-7.27049700	-0.08415200
N	-11.45045400	-1.18414300	-0.73078600
N	-6.65457300	4.66903800	1.38593800
N	6.64449500	4.82654800	-0.78047700
N	11.47529600	-1.31235900	0.07317000
C	7.92338600	5.44922900	-1.04657900
H	7.79835400	6.53412300	-1.06857300
H	8.62356200	5.19732100	-0.24487800
H	8.35733500	5.11956000	-2.00388000
C	5.50149000	5.43299500	-1.43801700
H	4.57408500	5.04071000	-1.01666500
H	5.52114000	6.51152900	-1.26137100
H	5.49411600	5.25782600	-2.52522300
C	-12.40475700	-0.19088000	-0.28646300
H	-12.18143300	0.76747200	-0.76383500
H	-13.40976300	-0.49848400	-0.58390700
H	-12.38259200	-0.04873900	0.80574300
C	-11.87563100	-2.56498300	-0.59449800
H	-12.87733800	-2.67152300	-1.01878000
H	-11.20456400	-3.22121800	-1.15193700

H	-11.90431500	-2.90099400	0.45404300
C	-5.52598800	5.52919500	1.08101000
H	-5.55771900	6.40255100	1.73749100
H	-4.58948000	5.00112200	1.27098300
H	-5.52561100	5.87841200	0.03640200
C	-7.94060900	5.32765400	1.46076700
H	-8.62804600	4.71413700	2.05029000
H	-7.82334500	6.29252700	1.95936600
H	-8.38647300	5.49126700	0.46661900
C	12.42879200	-0.23303300	-0.07072300
H	12.16642200	0.36852200	-0.94546500
H	12.45064900	0.42624000	0.81140500
H	13.42556900	-0.65220800	-0.22492200
C	11.93099700	-2.45209400	0.84757500
H	12.01936500	-2.22825700	1.92236000
H	11.24317400	-3.29035300	0.72229100
H	12.91114900	-2.76430000	0.47791500

Allene 19 M062X/6-31G*

0 1

C	-1.59012600	0.84949600	0.75380600
C	-1.22580300	-0.52092100	0.33776000
C	0.04377300	-0.92602700	0.40005400
C	-0.76045200	1.91331400	0.56684900
C	1.27533600	-0.41123000	0.44316100
C	0.62546300	1.95944400	0.07889000
C	1.53941700	0.94785500	-0.06712500
C	-2.46450600	-1.22002100	-0.03303200
H	-2.47454100	-2.22126000	-0.44747000
C	-3.52070300	-0.44736400	0.33064400
C	-3.04156200	0.84256600	0.86585400
C	2.98639000	1.02343400	-0.21887700
C	2.56215100	-1.00579300	0.83363400
H	2.64365000	-1.97732400	1.30637500
C	3.55796500	-0.19798900	0.38840200
C	0.93668300	3.37722100	-0.14038600
H	1.89469800	3.71663600	-0.51527700
C	-0.09548300	4.15872400	0.20165600
H	-0.11612600	5.24081100	0.14246500
C	-1.25007100	3.33944800	0.70481000
H	-2.17349800	3.49896300	0.12894300
H	-1.49219500	3.57751200	1.74988900
C	-4.12402600	1.60683800	1.14859200
H	-4.14945900	2.60918300	1.56179100
C	4.01706700	1.81445800	-0.60381500
H	3.97912800	2.78077500	-1.09402300
C	5.27855100	1.12827300	-0.28359000
C	5.00795500	-0.09815600	0.31416100
C	-4.97574300	-0.41471200	0.32917700
C	-5.33464400	0.83256400	0.82903800
C	5.95132800	-1.03512200	0.85101200

C	6.55476200	1.71643800	-0.58382600
H	6.51715000	2.72395600	-0.99608900
C	-5.84519800	-1.49807100	-0.02716000
C	-6.65207900	1.36389200	1.04734300
H	-6.68606700	2.34601700	1.51730900
C	7.31802700	-1.07035800	0.72212400
C	8.17575400	-0.19123100	-0.06962700
C	7.78206600	1.14743500	-0.48730600
C	-7.21165300	-1.51580400	-0.15973600
C	-8.14673600	-0.39800800	-0.04735000
C	-7.84194100	0.83148400	0.67308000
C	9.47677300	-0.44426900	-0.46421700
C	10.09216200	0.76788000	-0.99642600
C	-7.62791200	-2.91405400	-0.37042000
H	-8.66125600	-3.23312500	-0.43318300
C	-6.55370300	-3.71701800	-0.42506700
H	-6.55493100	-4.79037700	-0.56755800
C	-9.44688100	-0.35971000	-0.51619600
C	-10.14711700	0.80412200	0.01898200
C	9.03418400	1.84961900	-0.96185500
H	8.89350600	2.32246600	-1.93952600
H	9.32386500	2.64121100	-0.25840300
C	-9.14831000	1.56951000	0.86023000
H	-9.07344000	2.62019500	0.56052200
H	-9.45164600	1.55518800	1.91524200
C	-5.31656600	-2.89517200	-0.23708000
H	-4.71533500	-3.23071200	0.61886900
H	-4.65934900	-2.93759300	-1.11784800
C	5.51932800	-2.15470500	1.76528800
H	4.93132500	-1.77905600	2.61370100
H	4.87834800	-2.87142600	1.23131700
C	7.82852200	-2.13879200	1.59955800
H	8.88154900	-2.34160600	1.75312600
C	6.81079700	-2.77605000	2.19914000
H	6.88487200	-3.59818600	2.89986500
C	10.10426900	-1.75624300	-0.49833800
H	9.42984000	-2.58852100	-0.31408500
C	-10.00508600	-1.25344600	-1.51877900
H	-9.28149300	-1.90340300	-2.00403200
C	-11.27306400	-1.33873900	-1.97546500
H	-11.44378900	-2.07432300	-2.75841900
C	-12.45326600	-0.58380500	-1.58918400
H	-13.38564800	-0.92893400	-2.02883200
C	11.38014700	-2.08473300	-0.79383900
H	11.60834800	-3.14832300	-0.78398500
C	12.50406700	-1.23075300	-1.13952600
H	13.46228300	-1.73819200	-1.21740100
C	11.35971400	1.00243100	-1.40085600
H	11.58133500	2.01674400	-1.72820000
C	12.48706400	0.09076100	-1.41333900
H	13.43723300	0.54488200	-1.68622900
C	-11.44015100	1.17854800	-0.09532200

H	-11.72774800	2.08442300	0.43544900
C	-12.51705200	0.50489200	-0.79402900
H	-13.49990000	0.94929300	-0.65316700

PROTONATED

Allene 1H M062X/6-31G*

1 1			
C	-1.44898200	-0.69769600	0.00000000
C	-1.44898200	0.69769600	0.00000000
C	-0.35792500	1.56785500	0.00000000
C	-0.35792500	-1.56785500	0.00000000
C	1.00280100	1.25733300	0.00000000
C	1.00280100	-1.25733300	0.00000000
C	1.60843200	0.00000000	0.00000000
H	-2.42876800	-1.16944100	0.00000000
H	-2.42876800	1.16944100	0.00000000
H	-0.60008200	2.62780900	0.00000000
H	-0.60008200	-2.62780900	0.00000000
H	1.68033300	2.10761800	0.00000000
H	1.68033300	-2.10761800	0.00000000
H	2.69571500	0.00000000	0.00000000

Allene 2H M062X/6-31G*

1 1			
C	-0.50165500	-0.69320400	-0.00002000
C	-0.49522900	0.73067100	-0.00000100
C	0.61374600	1.59031800	-0.00002000
C	0.56611200	-1.57075200	-0.00004100
C	1.95710500	1.24976300	0.00000100
C	1.93644400	-1.26835600	-0.00000100
C	2.54875700	-0.02360800	0.00002900
H	0.38749700	2.65433200	-0.00004800
H	0.31475800	-2.62992900	-0.00006300
H	2.65221700	2.08567300	-0.00000400
H	2.60460500	-2.12554500	0.00000700
H	3.63559700	-0.03247400	0.00006500
C	-1.87177900	1.19362900	0.00001600
H	-2.15463300	2.23959500	0.00003200
C	-2.70494500	0.13341000	0.00000500
H	-3.78795600	0.17734300	0.00002900
C	-1.93682000	-1.14762200	0.00001900
H	-2.16126300	-1.76724600	-0.87960800
H	-2.16123700	-1.76723600	0.87966000

Allene 3H M062X/6-31G*

1 1			
C	0.66362700	-0.14054100	-0.00001800

C	1.39748600	1.08085600	-0.00003600
C	2.78764100	1.26259100	-0.00001800
C	1.15275000	-1.43337600	0.00000900
C	2.48720800	-1.86457500	0.00002200
C	3.64685500	-1.10302300	0.00002100
H	3.12753900	2.29586100	-0.00002700
H	0.40640000	-2.22609300	0.00001900
H	2.63009400	-2.94199700	0.00003700
H	4.57907900	-1.66136900	0.00003500
C	0.44631200	2.17559700	-0.00007100
H	0.73181200	3.22083200	-0.00009100
C	-0.80549700	1.67743000	-0.00007400
H	-1.71105500	2.27405000	-0.00010100
C	-0.81614600	0.17594400	-0.00002800
C	-1.51546300	-0.38973800	1.27065800
H	-1.04211200	0.03027200	2.16464900
H	-1.35372500	-1.47521700	1.29402500
C	-1.51550900	-0.38984400	-1.27063300
H	-1.04219600	0.03008900	-2.16467900
H	-1.35377200	-1.47532500	-1.29391600
C	-3.02086200	-0.11409600	1.26118900
H	-3.46370400	-0.56167400	2.15615400
H	-3.20533400	0.96554000	1.33262900
C	-3.02090900	-0.11420400	-1.26113100
H	-3.46378400	-0.56185900	-2.15604000
H	-3.20538500	0.96542500	-1.33265700
C	-3.68105300	-0.67222700	0.00006500
H	-3.59277300	-1.76718600	0.00011100
H	-4.75010400	-0.44175700	0.00007500
C	3.77845900	0.29331100	0.00000600
H	4.79961800	0.66576800	0.00001300

Allene 4H M062X/6-31G*

1 1			
C	-0.50166100	-0.69321000	0.00000200
C	-0.49522600	0.73066600	0.00000100
C	0.61375000	1.59031500	-0.00000100
C	0.56611100	-1.57075200	0.00000100
C	1.95710800	1.24976400	-0.00000200
C	1.93644200	-1.26835700	0.00000000
C	2.54875700	-0.02361000	-0.00000200
H	2.65222300	2.08567200	-0.00000300
H	3.63559700	-0.03247600	-0.00000200
C	-1.87177300	1.19363200	-0.00000100
H	-2.15462500	2.23959900	-0.00000400
C	-2.70494400	0.13341700	0.00000400
H	-3.78795600	0.17735000	0.00000400
C	-1.93682500	-1.14761700	0.00000000
H	-2.16126300	-1.76724000	-0.87963100
H	-2.16126200	-1.76724000	0.87963100
H	0.38749300	2.65432800	-0.00000200

H	0.31475900	-2.62993100	0.00000200
H	2.60460200	-2.12554600	0.00000000

Allene 5H M062X/6-31G*

1	1		
C	-0.66363100	-0.14054300	-0.00002300
C	-1.39748200	1.08085500	-0.00004500
C	-2.78763600	1.26259900	-0.00002300
C	-1.15275300	-1.43338000	0.00000900
C	-3.77845700	0.29332000	0.00000800
C	-2.48721300	-1.86457300	0.00002400
C	-3.64685700	-1.10301400	0.00002400
H	-0.40640400	-2.22609700	0.00002100
H	-4.79961600	0.66577900	0.00001800
H	-2.63010700	-2.94199400	0.00004100
H	-4.57908200	-1.66135700	0.00004100
C	-0.44630200	2.17559300	-0.00008900
H	-0.73180300	3.22082900	-0.00011300
C	0.80550400	1.67742200	-0.00009100
H	1.71106700	2.27403600	-0.00012300
C	0.81614800	0.17593200	-0.00003400
C	1.51551100	-0.38986300	-1.27063000
H	1.04220000	0.03005700	-2.16468300
H	1.35379400	-1.47534700	-1.29390400
C	1.51545300	-0.38973300	1.27066300
H	1.04209400	0.03028100	2.16464700
H	1.35373400	-1.47521400	1.29403900
C	3.02091200	-0.11421100	-1.26112600
H	3.20537800	0.96541800	-1.33266000
H	3.46379400	-0.56187500	-2.15602800
C	3.68105100	-0.67221900	0.00008200
C	3.02085200	-0.11407900	1.26120200
H	3.20531400	0.96555800	1.33263000
H	3.46369200	-0.56164800	2.15617200
H	4.75010200	-0.44174700	0.00009500
H	3.59277000	-1.76717800	0.00013800
H	-3.12753200	2.29586900	-0.00003400

Allene 6H M062X/6-31G*

1	1		
C	-0.67586400	-0.56836700	0.00002200
C	-1.56427200	0.55065700	-0.00004900
C	-1.27469300	1.89782300	-0.00008100
C	0.71506300	-0.54413600	0.00002000
C	-0.01316600	2.52319700	-0.00005600
C	1.57501600	0.57878900	-0.00000700
C	1.24197700	1.94738800	-0.00002000
H	-2.13143600	2.56894500	-0.00012200
H	2.08527000	2.63414900	-0.00000300
C	-2.97594900	0.02032400	-0.00006200

H	-3.53492900	0.36700400	-0.88003500
C	-2.78745700	-1.46285500	0.00004400
H	-3.61180900	-2.16664000	0.00007900
C	-1.48043700	-1.78390700	0.00005100
H	-1.06853800	-2.78576600	0.00009500
C	1.56688500	-1.78586200	0.00008300
H	1.36672300	-2.41201900	0.88097400
H	1.36666900	-2.41219400	-0.88066300
C	2.95118600	0.09912500	0.00003500
H	3.81430000	0.75406800	0.00004700
C	2.96168400	-1.24672100	0.00000800
H	3.84285100	-1.87733300	0.00000600
H	-0.03387600	3.60989500	-0.00007000
H	-3.53504500	0.36715800	0.87977100

Allene 7H M062X/6-31G*

1 1

C	-1.19849700	0.77451900	-0.00000200
C	-1.47270500	2.16763700	-0.00015000
C	-0.59480800	3.26594600	-0.00029500
C	0.06024600	0.16734300	0.00004900
C	0.78393100	3.26112000	-0.00035100
C	1.34182000	0.81258000	-0.00008200
C	1.64975300	2.15595000	-0.00026400
H	-1.07307900	4.24284700	-0.00038300
H	2.71059700	2.39868100	-0.00034200
C	-2.91446900	2.35263200	-0.00011600
H	-3.39210500	3.32545200	-0.00019700
C	-3.51831400	1.15368000	0.00002400
H	-4.59022100	0.99159300	0.00007300
C	-2.52537700	0.02555000	0.00007600
C	-2.71405700	-0.82980100	1.28808700
H	-2.68024200	-0.16605200	2.15904100
H	-1.87675900	-1.52716000	1.39106500
C	-2.71410400	-0.82995600	-1.28782500
H	-2.68031800	-0.16631200	-2.15886000
H	-1.87681300	-1.52732900	-1.39074800
C	-4.01938000	-1.62930600	1.25992000
H	-4.06667200	-2.25343300	2.15757900
H	-4.88095700	-0.95141700	1.30928400
C	-4.01942700	-1.62945600	-1.25952100
H	-4.06675100	-2.25368600	-2.15710600
H	-4.88100300	-0.95156800	-1.30893400
C	-4.11650100	-2.49061000	0.00025200
H	-3.30091600	-3.22794600	0.00028100
H	-5.05236600	-3.05681100	0.00030300
C	2.43602700	-0.23863800	-0.00000200
C	0.31379700	-1.27298700	0.00025300
H	-0.45072400	-2.03579700	0.00040700
C	1.63695400	-1.50642800	0.00022800
H	2.08917200	-2.49215000	0.00035900

C	3.32736300	-0.13044000	1.26839900
H	2.70220500	-0.23169500	2.16237600
C	3.32716200	-0.13080500	-1.26858100
H	2.70185800	-0.23232400	-2.16242500
C	4.45490800	-1.16542400	-1.26290300
H	4.03590000	-2.17719800	-1.33838700
H	5.07067200	-1.02037600	-2.15600600
C	4.45510600	-1.16506400	1.26284000
H	5.07101100	-1.01976100	2.15580500
H	4.03610600	-2.17681300	1.33867600
C	5.31009000	-1.04875900	-0.00011500
H	5.82021800	-0.07577500	-0.00029500
H	6.09117600	-1.81462800	-0.00006700
H	3.76917800	0.87421600	1.29302700
H	3.76896600	0.87384600	-1.29357200
H	1.26477200	4.23588300	-0.00048300

Allene 8H M062X/6-31G*

1 1

C	-0.71512800	-0.54420100	0.00000600
C	-1.57496800	0.57885100	-0.00000700
C	-1.24191600	1.94746200	-0.00003000
C	0.67583400	-0.56842100	0.00001400
C	0.01325400	2.52326400	-0.00003900
C	1.56425900	0.55060000	0.00000500
C	1.27469800	1.89781400	-0.00002100
H	0.03400000	3.60995300	-0.00005700
H	2.13155300	2.56878100	-0.00002600
C	-2.95116100	0.09919700	-0.00001600
H	-3.81437200	0.75399600	-0.00003400
C	-2.96171300	-1.24670600	0.00002200
H	-3.84296800	-1.87717100	0.00002700
C	-1.56698200	-1.78587600	0.00000100
H	-1.36673600	-2.41211600	-0.88082700
H	-1.36673100	-2.41210800	0.88083300
C	2.97595900	0.02028400	0.00001000
H	3.53499700	0.36704700	-0.87991300
H	3.53499600	0.36708000	0.87991800
C	1.48039500	-1.78394000	0.00001500
H	1.06873700	-2.78589100	0.00000900
C	2.78747300	-1.46283300	0.00004900
H	3.61174300	-2.16670300	0.00006300
H	-2.08523300	2.63417100	-0.00004200

Allene 9H M062X/6-31G*

1 1

C	-1.19849700	0.77451900	-0.00001000
C	-1.47270600	2.16763700	-0.00010500
C	0.06024600	0.16734300	0.00003500
C	0.78393100	3.26112000	-0.00023600

C	1.34182000	0.81258000	-0.00004600
C	1.64975300	2.15595000	-0.00017100
H	1.26477200	4.23588300	-0.00032100
H	2.71059700	2.39868100	-0.00021600
C	-2.91447000	2.35263200	-0.00005900
H	-3.39210600	3.32545200	-0.00009600
C	-3.51831400	1.15367900	0.00004000
H	-4.59022200	0.99159300	0.00008900
C	-2.52537600	0.02555000	0.00002900
C	0.31379700	-1.27298700	0.00020000
H	-0.45072400	-2.03579600	0.00031800
C	1.63695400	-1.50642800	0.00019000
H	2.08917200	-2.49215000	0.00029500
C	4.45506700	-1.16510800	1.26289300
H	5.07094500	-1.01983800	2.15588200
H	4.03606700	-2.17686100	1.33868100
C	5.31009000	-1.04875900	-0.00003200
H	6.09117600	-1.81462800	0.00001300
H	5.82021800	-0.07577400	-0.00016100
C	4.45494600	-1.16537900	-1.26284900
H	5.07073700	-1.02029900	-2.15592900
H	4.03594000	-2.17714900	-1.33838100
C	3.32732400	-0.13048600	1.26845600
H	2.70213700	-0.23177500	2.16240800
H	3.76913600	0.87417000	1.29313500
C	3.32720100	-0.13075900	-1.26852500
H	3.76900800	0.87389200	-1.29346500
H	2.70192500	-0.23224400	-2.16239300
C	2.43602700	-0.23863800	0.00002200
C	-4.01944000	-1.62938900	-1.25964000
H	-4.88101700	-0.95149900	-1.30900800
H	-4.06677400	-2.25357100	-2.15725800
C	-4.01936700	-1.62937400	1.25980000
H	-4.06664900	-2.25354800	2.15742700
H	-4.88094300	-0.95148700	1.30920900
C	-2.71411700	-0.82988600	-1.28791700
H	-1.87682800	-1.52725400	-1.39089100
H	-2.68034200	-0.16619500	-2.15891600
C	-2.71404300	-0.82986900	1.28799500
H	-2.68021800	-0.16616800	2.15898400
H	-1.87674400	-1.52723400	1.39092600
C	-4.11650000	-2.49061000	0.00008700
H	-5.05236500	-3.05681300	0.00011800
H	-3.30091400	-3.22794500	0.00006900
C	-0.59480800	3.26594600	-0.00020000
H	-1.07307900	4.24284700	-0.00025500

Allene 10H M062X/6-31G*

1 1			
C	-0.00002800	1.55700300	-0.68148900
C	0.00001800	1.25037800	0.71517900

C	0.00000000	0.00000000	1.33093500
C	-0.00001800	0.70392600	-1.76280300
C	-0.00001800	-1.25037800	0.71517900
C	0.00001800	-0.70392600	-1.76280300
C	0.00002800	-1.55700300	-0.68148900
H	-0.00000900	1.17422400	-2.74451600
H	0.00000900	-1.17422400	-2.74451600
C	-0.00010000	2.50705300	1.45119300
H	-0.00017200	2.56650500	2.53311000
C	0.00002800	3.54117200	0.58943800
H	0.00004700	4.59105400	0.85870000
C	-0.00002800	3.05808900	-0.82545300
H	-0.88007400	3.40698300	-1.38304300
H	0.87991500	3.40702700	-1.38316200
C	0.00002800	-3.05808900	-0.82545300
H	-0.87991500	-3.40702700	-1.38316200
H	0.88007400	-3.40698300	-1.38304300
C	0.00010000	-2.50705300	1.45119300
H	0.00017200	-2.56650500	2.53311000
C	-0.00002800	-3.54117200	0.58943800
H	-0.00004700	-4.59105400	0.85870000
H	0.00000000	0.00000000	2.41941400

Allene 11H M062X/6-31G*

1 1

C	-1.56148900	0.00699300	0.00000400
C	-1.22248600	-1.38494100	-0.00002000
C	0.03349600	-1.97635100	-0.00002500
C	-0.72348000	1.09372400	-0.00000100
C	1.28055900	-1.34207900	0.00001200
C	0.70845200	1.12126100	-0.00001200
C	1.58214500	0.04550000	0.00001000
C	-2.46758700	-2.14747800	-0.00005500
H	-2.50248300	-3.23052000	-0.00009200
C	-3.51878200	-1.31128800	-0.00001600
H	-4.56272700	-1.60226600	-0.00001200
C	-3.06740000	0.11789100	0.00006500
H	-3.43281000	0.66406500	-0.88022800
H	-3.43274900	0.66394900	0.88045800
C	3.08239700	0.19866300	0.00001400
H	3.43208400	0.75464900	-0.88099100
H	3.43212000	0.75477300	0.88091800
C	2.54146600	-2.07735800	0.00002500
H	2.60132100	-3.15930800	0.00001800
C	3.57293700	-1.21502400	0.00006100
H	4.62398100	-1.47898800	0.00009600
C	1.12895200	2.52140000	-0.00008400
H	2.16334800	2.84337500	-0.00013600
C	0.05117700	3.32278500	-0.00003300
H	0.06672100	4.40641300	-0.00006400
C	-1.21518400	2.52199500	0.00003400

H	-1.83605300	2.73711800	-0.88011300
H	-1.83585400	2.73708400	0.88033600
H	0.05206200	-3.06450400	-0.00006100

Allene 12H M062X/6-31G*

1	1		
C	-1.59481300	0.07737800	-0.00001000
C	-1.28050800	-1.29678300	0.00005000
C	-0.03941100	-1.93192900	0.00006600
C	-0.69560300	1.16777700	-0.00002300
C	1.21642900	-1.35145600	0.00002400
C	0.71278800	1.12897600	-0.00002600
C	1.56768400	0.02428300	-0.00002000
C	-2.57175300	-2.07258700	0.00009300
H	-2.64401600	-2.72709100	0.87985300
C	-3.61801000	-1.00742900	-0.00000400
H	-4.68143300	-1.21391600	-0.00002700
C	-3.04939300	0.21183600	-0.00002600
C	3.02599800	0.11702500	-0.00003100
C	2.48902600	-2.15995500	0.00002200
H	2.54847900	-2.81514800	0.87984100
C	3.56032400	-1.11719700	-0.00003400
H	4.61839600	-1.35066200	-0.00005600
H	2.54844800	-2.81524700	-0.87972300
H	-2.64401000	-2.72736500	-0.87945400
H	-3.57675000	1.15683800	-0.00006500
H	3.57569900	1.05029300	-0.00004800
C	-1.11316000	2.56822000	-0.00003600
H	-2.14349600	2.89900200	-0.00003100
C	-0.02988600	3.36400600	-0.00004900
H	-0.03507100	4.44731100	-0.00005900
C	1.22115000	2.54712300	-0.00004000
H	1.84639200	2.75091500	0.88050200
H	1.84641000	2.75090500	-0.88057000
H	-0.06422100	-3.02155800	0.00010200

Allene 13H M062X/6-31G*

1	1		
C	0.66440300	2.49536700	0.26806900
C	1.50781600	1.44864300	0.41336200
C	1.27670400	0.05620500	0.06711400
C	-0.66451700	2.49531000	-0.26801400
C	0.00007300	-0.53424000	0.00003600
C	-1.50783500	1.44851200	-0.41331000
C	-1.27661200	0.05610400	-0.06705900
H	1.05465600	3.46936100	0.55061600
H	2.48373600	1.67852100	0.82391400
H	-1.05486800	3.46927400	-0.55052900
H	-2.48381700	1.67829100	-0.82378800
N	2.36708100	-0.72282300	-0.07584000

N	-2.36703100	-0.72287600	0.07583100
C	3.72229300	-0.17141800	-0.00214300
H	4.01116200	0.05700900	1.02935600
H	4.41782200	-0.90873100	-0.39780500
H	3.80412600	0.73039500	-0.61281600
C	2.23305100	-2.15693300	-0.31284200
H	1.76696600	-2.65610200	0.54416300
H	1.63455800	-2.34649100	-1.20989800
H	3.22167400	-2.58591100	-0.45945000
C	-3.72214700	-0.17128500	0.00188400
H	-3.80389300	0.73064800	0.61239400
H	-4.01084900	0.05702900	-1.02968700
H	-4.41784500	-0.90842100	0.39757900
C	-2.23322800	-2.15699000	0.31296500
H	-1.76706000	-2.65629000	-0.54391800
H	-1.63493700	-2.34657400	1.21014900
H	-3.22193800	-2.58581700	0.45942200
H	0.00014600	-1.61193500	-0.00000500

Allene 14H M062X/6-31G*

1 1

C	0.67040600	1.67081600	0.16031100
C	1.58666300	0.62175300	0.12446800
C	1.30154600	-0.76682900	-0.05406200
C	-0.74212500	1.64903300	0.00661800
C	0.00760000	-1.34533800	-0.04546600
C	-1.60714900	0.58007000	-0.10831900
C	-1.28496400	-0.82510600	0.01285200
C	2.97317600	1.22872400	0.08081600
H	3.49802200	0.92568900	-0.83627300
C	2.72169200	2.69910300	0.13212900
H	3.51428400	3.43744500	0.14289800
C	1.40501900	2.93935400	0.19762900
H	0.93137300	3.91122500	0.25826800
C	-1.52885400	2.91908100	-0.20094000
H	-1.50105800	3.55944300	0.69219000
H	-1.11783400	3.51710600	-1.02567100
C	-2.94022600	1.09118800	-0.45342700
H	-3.79441800	0.46550800	-0.67466100
C	-2.90662600	2.43231000	-0.50494700
H	-3.73484300	3.08468300	-0.75194600
H	0.04172500	-2.42224500	0.03775800
H	3.61653600	0.93715400	0.91693300
N	-2.33652500	-1.69302600	0.12332000
N	2.33881400	-1.64880700	-0.20524300
C	-2.17456600	-3.11063600	-0.16010300
H	-1.69245200	-3.65194500	0.66621700
H	-3.16740500	-3.53812200	-0.31430000
H	-1.59692600	-3.25027700	-1.07637100
C	2.13460800	-2.92930600	-0.86998000
H	3.08572300	-3.23745900	-1.31045000

H	1.80741400	-3.71681000	-0.17621200
H	1.40370700	-2.82452300	-1.67341300
C	3.56775400	-1.59068600	0.58759100
H	3.83009800	-2.61220300	0.87513500
H	4.40826500	-1.16504100	0.03069000
H	3.40511600	-1.02670700	1.50592700
C	-3.46628800	-1.41708600	1.01490400
H	-4.41744400	-1.50316100	0.48077600
H	-3.45712900	-2.15041700	1.82972400
H	-3.38477000	-0.42517100	1.45580800

Allene 15H M062X/6-31G*

1 1

C	-1.58240200	-0.11623300	0.22787600
C	-1.24326100	1.30233100	0.19972400
C	0.00340300	1.91344400	0.24547900
C	-0.69835600	-1.15636800	0.51209600
C	1.26899200	1.33232500	0.23800700
C	0.72742300	-1.11891500	0.62066400
C	1.60686800	-0.07390400	0.30864600
C	-2.44611800	2.05317700	0.11561200
H	-2.47405500	3.13422100	0.09594900
C	-3.52422600	1.20202000	0.03980100
C	-3.03450300	-0.18134600	0.07189400
C	3.04729000	-0.15627100	0.14636400
C	2.47216100	2.08158900	0.16688000
C	3.54915400	1.21992600	0.10973400
C	1.16600100	-2.41440700	1.16194900
H	2.18071700	-2.62351400	1.47084700
C	0.12152500	-3.23393600	1.32436000
H	0.14759800	-4.23288100	1.74243400
C	-1.13200400	-2.57180600	0.85123700
H	-1.93422500	-2.59487200	1.59777200
H	-1.50085500	-3.09677200	-0.04058400
C	-3.78259000	-1.32850800	-0.11370800
H	-3.24038400	-2.26468700	-0.15133100
C	-5.16480800	-1.48065200	-0.29254300
C	-6.17524600	-0.51732300	-0.32029300
C	-4.89062300	1.63785100	-0.05276600
C	-6.04471400	0.88681300	-0.19975800
H	2.50773100	3.16209200	0.12790300
C	4.92023800	1.63001600	0.01942500
C	6.05600900	0.85449700	-0.16311700
C	3.75092300	-1.31506300	-0.13839500
H	3.16226300	-2.22332700	-0.23842700
C	5.11995500	-1.48891300	-0.36277700
C	6.15171700	-0.54276200	-0.35406800
C	5.33324900	3.03271300	0.11494100
H	4.64944600	3.85758900	0.26949300
C	6.66860900	3.12261600	0.00034500
H	7.25586300	4.03188600	0.04052300

C	7.41200000	-1.24031600	-0.61312700
H	8.37795900	-0.75116800	-0.65712600
C	7.17983300	-2.55335100	-0.78775400
H	7.92612000	-3.31106800	-0.99424100
C	-5.27032200	3.05301600	0.00018000
H	-4.56806900	3.86795600	0.11899000
C	-6.60382000	3.17136000	-0.10937400
H	-7.16897300	4.09525600	-0.09797100
C	-7.45493700	-1.20004900	-0.51629500
H	-8.41069100	-0.69254500	-0.57382600
C	-7.25368100	-2.52603600	-0.61436900
H	-8.01825100	-3.27872200	-0.76379400
C	-7.22731300	1.82011500	-0.25100400
H	-7.77892100	1.72385300	-1.19670100
H	-7.94759300	1.61343200	0.55277100
C	-5.79721600	-2.83797800	-0.48838500
H	-5.59623000	-3.51117200	0.35650700
H	-5.41188700	-3.34097100	-1.38644400
C	5.71904900	-2.84322900	-0.65773900
H	5.51618600	-3.56821100	0.14240900
H	5.30853100	-3.27552500	-1.58103800
C	7.25954900	1.76295000	-0.19274900
H	7.98169200	1.51256600	0.59683300
H	7.80082900	1.68766200	-1.14617800
H	-0.01164700	3.00255600	0.23327500

Allene 16H M062X/6-31G*

1 1

C	-1.57222200	0.35107600	-0.00001000
C	-1.24222900	-1.09430900	-0.00002300
C	0.01905800	-1.68670400	-0.00003200
C	-0.73665200	1.41699000	-0.00000600
C	1.26066200	-1.06696500	-0.00002800
C	0.72766600	1.43892000	-0.00001000
C	1.58977500	0.37838900	-0.00001400
C	-2.44310400	-1.82617100	-0.00002700
H	-2.48917000	-2.91042400	-0.00003600
C	-3.52481700	-0.93552400	-0.00001500
C	-3.03065600	0.40714900	-0.00000400
C	3.04472200	0.43518300	-0.00000900
C	2.47031300	-1.80083800	-0.00004200
H	2.51728300	-2.88495100	-0.00005600
C	3.53989800	-0.91142700	-0.00003000
C	1.12275700	2.84767700	-0.00000800
H	2.15010200	3.18393100	-0.00001600
C	0.04509200	3.64477500	-0.00000200
H	0.06450400	4.72842700	-0.00000200
C	-1.22733100	2.84853100	0.00000300
H	-1.84676400	3.06150200	-0.88187900
H	-1.84675200	3.06149400	0.88189600
C	-4.09313700	1.29771000	0.00001800

H	-4.06713800	2.37962500	0.00003100
C	4.12219600	1.31496000	0.00002500
H	4.11506400	2.39649400	0.00004900
C	5.31627600	0.54972300	0.00002200
C	4.96575200	-0.88101000	-0.00000700
C	-4.94392000	-0.89942600	0.00000100
C	-5.29463800	0.53453900	0.00001000
C	5.80683500	-1.97592600	-0.00001800
H	5.31605600	-2.94779400	-0.00004700
C	-5.79506900	-1.99303200	-0.00000200
H	-5.30854500	-2.96708700	-0.00001500
C	-7.19134800	-2.01104400	0.00000500
H	-7.64891700	-2.99630000	0.00000000
C	-8.07275300	-0.93407200	0.00001500
H	-9.12741400	-1.19805200	0.00001900
C	7.20849400	-2.00152200	0.00000000
H	7.65961800	-2.98977000	-0.00001400
C	8.09121500	-0.93245000	0.00003000
H	9.14527400	-1.19849200	0.00003900
C	6.60370700	1.09965800	0.00004700
H	6.64494600	2.18734200	0.00006800
C	7.82540500	0.44600100	0.00005100
H	8.70156700	1.08819000	0.00007300
C	-6.57481800	1.08784900	0.00001900
H	-6.61212800	2.17577000	0.00002900
C	-7.80424500	0.43822300	0.00002200
H	-8.67696200	1.08494900	0.00003000
H	0.03207500	-2.77646100	-0.00004300

Allene 17H M062X/6-31G*

1 1			
C	-1.57427200	-0.82399200	0.00000000
C	-1.24441000	0.61989500	-0.00000500
C	0.01673800	1.20958900	-0.00000600
C	-0.73732000	-1.89007100	-0.00000100
C	1.25956300	0.59113500	-0.00000300
C	0.72468000	-1.91257100	-0.00000500
C	1.58827400	-0.85287300	-0.00000500
C	-2.44979200	1.34991300	-0.00000600
H	-2.48644200	2.43413500	-0.00001000
C	-3.53331600	0.46369200	-0.00000200
C	-3.03009100	-0.88191700	0.00000400
C	3.04264400	-0.91148100	-0.00001100
C	2.47193300	1.32301700	0.00000800
H	2.50814900	2.40707700	0.00001000
C	3.54580000	0.43867100	-0.00000800
C	1.11938400	-3.32257100	-0.00001200
H	2.14692900	-3.65827200	-0.00001900
C	0.04183400	-4.11933300	-0.00000800
H	0.06033000	-5.20297600	-0.00001100

C	-1.22950600	-3.32074500	0.00000100
H	-1.85103400	-3.53178900	0.88118000
H	-1.85104700	-3.53178800	-0.88117000
C	-4.08398100	-1.77605100	0.00001800
H	-4.05263600	-2.85784800	0.00002600
C	4.11072000	-1.79369700	-0.00002700
H	4.09968900	-2.87527600	-0.00003500
C	5.31403500	-1.03257400	0.00000500
C	4.97540800	0.39532800	-0.00003000
C	-4.95775500	0.41277100	0.00000600
C	-5.29409000	-1.01849100	0.00001700
C	5.84194000	1.47452800	-0.00004000
C	6.59000200	-1.60479800	0.00002000
H	6.61220000	-2.69463000	0.00002500
C	-5.83418000	1.48903200	0.00000000
C	-6.56424200	-1.59503800	0.00002900
H	-6.58187000	-2.68502100	0.00003800
C	7.26021200	1.49597600	-0.00002500
C	8.13837000	0.40751500	-0.00000300
C	7.82072500	-0.97682100	0.00001600
C	-7.24840000	1.50279200	0.00000800
C	-8.12347800	0.40716100	0.00002300
C	-7.80096900	-0.97217000	0.00003200
C	9.59869100	0.52767500	0.00000600
H	10.13085500	1.47048100	-0.00000300
C	10.16406200	-0.69029100	0.00002400
H	11.22750800	-0.89703200	0.00003300
C	-7.68405700	2.90490900	-0.00000600
H	-8.72050800	3.21806300	-0.00000500
C	-6.62090300	3.72094000	-0.00002000
H	-6.64572000	4.80360900	-0.00003200
C	-9.58426000	0.52268900	0.00002900
H	-10.11987900	1.46350900	0.00002300
C	-10.14495900	-0.69767100	0.00004800
H	-11.20745900	-0.90914600	0.00005800
C	9.11547000	-1.75709700	0.00002500
H	9.19103000	-2.41014200	0.87998900
H	9.19103700	-2.41015100	-0.87993300
C	-9.09120800	-1.75884300	0.00004700
H	-9.16392700	-2.41232100	0.88001000
H	-9.16393900	-2.41233100	-0.87990800
C	-5.35233300	2.92089100	-0.00001500
H	-4.73179700	3.12839400	-0.88218000
H	-4.73179500	3.12841200	0.88214500
C	5.35309800	2.90435600	-0.00004500
H	4.73169700	3.10923300	-0.88223000
H	4.73168800	3.10924300	0.88213100
C	7.68634400	2.90050500	-0.00003900
H	8.72077400	3.22025200	-0.00003500
C	6.61829100	3.71007500	-0.00004800
H	6.63748000	4.79290900	-0.00005400
H	0.03051200	2.29966600	-0.00000600

Allene 18H M062X/6-31G*

1 1

C	-1.57207700	-0.99414200	-0.03039500
C	-1.24609600	0.45068700	-0.03554200
C	0.02386900	1.03689000	-0.03950400
C	-0.73432500	-2.05743500	-0.03490700
C	1.25781300	0.41455600	-0.03729300
C	0.72804200	-2.09805200	-0.04172600
C	1.59081300	-1.02397800	-0.03389400
C	-2.45084900	1.17154300	-0.03578800
H	-2.48968900	2.25620100	-0.04050400
C	-3.53844500	0.28218800	-0.02949100
C	-3.02952900	-1.05925700	-0.02566600
C	3.03200200	-1.08427700	-0.02215500
C	2.48062400	1.15160400	-0.03373400
H	2.51374300	2.23598400	-0.03528000
C	3.54442200	0.26905100	-0.02434100
C	1.11868800	-3.48198200	-0.06379800
H	2.14403900	-3.81592600	-0.10323900
C	0.01906600	-4.29906600	-0.05073800
C	-1.24567100	-3.47814600	-0.03943800
H	-1.86042200	-3.68724300	0.84693300
H	-1.87378700	-3.67324700	-0.91954700
C	-4.08155600	-1.95696300	-0.01770700
H	-4.04858800	-3.03924700	-0.01196700
C	4.10421000	-1.96674400	-0.00206000
H	4.09018200	-3.04853600	0.01261500
C	5.30891000	-1.21053400	0.00619200
C	4.98365000	0.21287600	-0.00830700
C	-4.96244000	0.22367000	-0.02338200
C	-5.29493300	-1.20261800	-0.01506600
C	5.85270600	1.28469200	-0.00632600
C	6.59190100	-1.77794900	0.02686900
H	6.61854400	-2.86792300	0.03846600
C	-5.84797800	1.29614600	-0.02388800
C	-6.56852600	-1.77364200	-0.00297100
H	-6.59054400	-2.86407200	0.00451100
C	7.27197100	1.32923100	0.00589300
C	8.15645200	0.23590600	0.02674000
C	7.81487800	-1.14688600	0.03473300
C	-7.25659900	1.33140200	-0.01340200
C	-8.14250200	0.22691400	-0.00198000
C	-7.80029300	-1.14876100	0.00196300
C	9.59402500	0.36057600	0.05335600
H	10.12322800	1.30256200	0.07448900
C	10.17418600	-0.87975900	0.06159100
C	-7.69702900	2.71434000	-0.00790400
H	-8.73191400	3.02466200	0.01439100
C	-6.61595800	3.54541100	-0.03048500
C	-9.57748300	0.35450900	0.01496500

H	-10.10732900	1.29598300	0.03190700
C	-10.15809800	-0.88811100	0.01560300
C	9.10418300	-1.93926400	0.06378400
H	9.15971400	-2.57299500	0.95850400
H	9.18838900	-2.60142700	-0.80765200
C	-9.08618900	-1.94489300	0.02030400
H	-9.14866600	-2.58235700	0.91206500
H	-9.16545100	-2.60326300	-0.85457700
C	-5.35170200	2.72282800	-0.02845700
H	-4.73428900	2.92488800	-0.91333500
H	-4.73091000	2.92168000	0.85514600
C	5.34753700	2.70860300	-0.02734900
H	4.73712600	2.89291100	-0.92138600
H	4.71648900	2.91766800	0.84641100
C	7.69638200	2.71420700	-0.01342200
H	8.72875900	3.03345100	-0.02972900
C	6.60777000	3.53744000	-0.01870400
H	0.04006900	2.12727900	-0.04258200
N	0.00142800	-5.65005200	-0.02050500
C	1.26669400	-6.35308200	-0.11582100
H	1.10095700	-7.41601100	0.06599600
H	1.72778700	-6.22687400	-1.10477500
H	1.95640500	-5.97322500	0.64354000
C	-1.20314200	-6.40211600	-0.32237100
H	-1.16905600	-7.35992300	0.20246200
H	-2.08326000	-5.85878600	0.02373000
H	-1.30886700	-6.59629500	-1.39850500
N	-11.47636000	-1.18713900	-0.01286100
N	-6.59889600	4.90448800	-0.09261200
N	6.58205400	4.89579500	0.02152000
N	11.49460900	-1.18041500	0.03833500
C	-12.42451700	-0.09397900	0.08973400
H	-12.37929200	0.39241400	1.07378100
H	-12.21013700	0.65291800	-0.68038700
H	-13.43300800	-0.47740900	-0.07119900
C	-11.94772900	-2.52317600	0.30470000
H	-11.26611000	-3.27015500	-0.10519700
H	-12.03906800	-2.68452400	1.38778000
H	-12.92733800	-2.67461000	-0.15345600
C	-7.86953800	5.59097000	0.02838400
H	-7.72256700	6.65591300	-0.15905300
H	-8.56741600	5.20148400	-0.71850100
H	-8.31487100	5.46080300	1.02532200
C	-5.40898500	5.63722100	0.29787900
H	-4.51927000	5.15309600	-0.10982200
H	-5.46108600	6.64617200	-0.11716300
H	-5.29989700	5.71339400	1.38966500
C	5.39078800	5.61988700	-0.38109300
H	5.42957200	6.62819800	0.03715200
H	5.29527200	5.69819200	-1.47381900
H	4.50013500	5.12730800	0.01385100
C	7.84910900	5.59146000	-0.08653300

H	8.30837000	5.45798600	-1.07646300
H	7.69105200	6.65642800	0.09138800
H	8.53975800	5.21266000	0.67242200
C	11.96297500	-2.50864100	0.39087700
H	11.28491700	-3.26497400	-0.00769900
H	12.94628900	-2.67024200	-0.05599100
H	12.04590000	-2.64617900	1.47813800
C	12.43997300	-0.08596600	0.14566700
H	13.44966700	-0.46690200	-0.01464700
H	12.22530600	0.66180300	-0.62347400
H	12.39259800	0.39925200	1.13055600

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C	1.56440500	0.93760800	-0.10999000
C	1.22685900	-0.49793200	-0.08590600
C	0.00326800	-1.09727200	-0.03149000
C	0.69859100	2.01658200	-0.06963100
C	-1.28158400	-0.49318600	0.02692300
C	-0.71848200	2.03235100	0.00625100
C	-1.61719700	0.95644100	0.05134600
C	2.47964900	-1.23961200	-0.13899200
H	2.51674300	-2.32413400	-0.13442200
C	3.52004400	-0.36108800	-0.19356400
C	2.98664000	0.99483900	-0.18159400
C	-3.02327200	1.02323100	0.12090100
C	-2.45279200	-1.22827600	0.07730100
H	-2.49444600	-2.31048900	0.07034300
C	-3.54410900	-0.31342400	0.13374100
C	-1.13508500	3.43754000	0.02740200
H	-2.16556000	3.75924200	0.07913100
C	-0.06541300	4.24563900	-0.03006100
H	-0.08657300	5.32906100	-0.03059800
C	1.19628900	3.44102200	-0.09866700
H	1.86709800	3.65406000	0.74558000
H	1.76604900	3.65312900	-1.01442800
C	4.06174600	1.86299500	-0.25244800
H	4.04141900	2.94671300	-0.27854400
C	-4.12844000	1.93668400	0.19407100
H	-4.09788500	3.01761000	0.22508300
C	-5.29262300	1.20798700	0.23391500
C	-4.94328200	-0.26100300	0.19525800
C	4.96450500	-0.28073000	-0.25954500
C	5.27479400	1.10319500	-0.29957900
C	-5.81653600	-1.33888400	0.28037200
C	-6.59480900	1.75904000	0.32647100
H	-6.62705900	2.84621200	0.39700700
C	5.85290300	-1.37870300	-0.34632200
C	6.57641300	1.70712000	-0.40438000
H	6.57520000	2.79146800	-0.50517100
C	-7.22835700	-1.37201700	0.29527400

C	-8.12522800	-0.27798000	0.16943900
C	-7.80080800	1.12469400	0.29806000
C	7.24120900	-1.39782800	-0.32171400
C	8.15232800	-0.29072700	-0.13787900
C	7.78810700	1.10795800	-0.34195200
C	-9.52626800	-0.39540100	-0.07886200
C	-10.16520000	0.87945700	0.10320200
C	7.67207900	-2.77730300	-0.58942600
H	8.70411200	-3.07647400	-0.71781700
C	6.60368900	-3.58273300	-0.71208300
H	6.62240400	-4.64393300	-0.92789000
C	9.50758100	-0.38401700	0.17543700
C	10.15052100	0.90702700	0.00062900
C	-9.09359500	1.90547500	0.35193000
H	-9.23406200	2.38478300	1.32948900
H	-9.13857600	2.69980900	-0.40313400
C	9.07655100	1.89873900	-0.38553800
H	9.05338700	2.76002100	0.29068900
H	9.26060500	2.28631500	-1.39578700
C	5.35003900	-2.78663200	-0.54120500
H	4.68974800	-2.86836800	-1.41532700
H	4.76793100	-3.12258000	0.32917600
C	-5.30218500	-2.75409800	0.40165300
H	-4.74795700	-3.05136200	-0.49979900
H	-4.60910400	-2.86248500	1.24628100
C	-7.62657500	-2.76707500	0.53155500
H	-8.64224900	-3.09382900	0.71154600
C	-6.54547000	-3.56115900	0.59261300
H	-6.55062800	-4.62672700	0.78750600
C	-10.17648200	-1.54373800	-0.62401200
H	-9.51804800	-2.32947500	-0.97840200
C	10.15823000	-1.53680900	0.75907600
H	9.48952500	-2.32451800	1.09383100
C	11.47598500	-1.74287300	1.00363600
H	11.72206300	-2.69374000	1.47072200
C	12.60994300	-0.88763200	0.74941100
H	13.58148600	-1.33730300	0.93455600
C	-11.51493100	-1.77551100	-0.80165800
H	-11.76343100	-2.74063600	-1.23661700
C	-12.63310100	-0.95021700	-0.50091700
H	-13.60754500	-1.40659900	-0.64938300
C	-11.49669900	1.20130400	0.10369400
H	-11.72741000	2.24266100	0.32025100
C	-12.62130700	0.36102300	-0.10788600
H	-13.58958300	0.83568700	0.02659500
C	11.46083700	1.24880100	0.07872600
H	11.69583400	2.28919100	-0.13797000
C	12.59732900	0.41114900	0.36271800
H	13.56347000	0.89968300	0.26380900
H	-0.00117100	-2.18723000	-0.03053400

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