Palladium-Catalyzed Intramolecular Asymmetric Hydroamination, Hydroalkoxylation and Hydrocarbonation of Alkynes

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Page S-1: Title of the paper, author's name and address along with the contents.

Page S-2: General procedures

Page S-3: Catalytic Asymmetric Hydroamination of Alkynes

Page S-6: Catalytic Asymmetric Hydroalkoxylation of Alkynes

Page S-11: Catalytic Asymmetric Hydrocarbonation of Alkynes

Page S-15: ^1H NMR spectra of all compounds

Page S-50: Cartesian Coordinates

General

The ^1H NMR and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz, respectively, using CDCl_3 as solvent and were reported in ppm relative to CHCl_3 ($\delta = 7.26$) for ^1H NMR and relative to the central CDCl_3 ($\delta = 77.00$) resonance for ^{13}C NMR. Coupling constants in ^1H NMR are in Hz. Optical Rotations were measured on a digital polarimeter. HPLC was performed using a CHIRALCEL OD column (4.6 mm x 250 mm). $\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$ and benzoic acid were purchased. (*R,R*)-NORPHOS, biphenyl ligands **16**, **17** and **18** were purchased. (*R,R*)-RENORPHOS **4** was prepared from commercial available (*R,R*)-NORPHOS by hydrogenation with 10% Pd/C in methanol (see ref 35 in the text). Unless otherwise noted all experiments were carried out using (*R,R*)-RENORPHOS.

General procedures for asymmetric intramolecular hydroamination, hydroalkoxylation and hydrocarbonation reactions

Conditions A: To $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (5 mol%), PhCOOH (10 mol%) and (*R,R*)-RENORPHOS³⁵ (25 mol%) was added a substrate (0.125 mmol) in 1.5 ml of benzene under Ar atmosphere in a screw capped vial. After heating at 100°C for 72 h, the reaction mixture was filtered through a short silica gel column using diethyl ether as an eluent. After evaporation of the solvent, the residue was purified by silica gel column chromatography to afford the corresponding cyclization product.

Conditions B: To $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (20 mol%), PhCOOH (40 mol%) and (*R,R*)-RENORPHOS (100 mol%) was added a substrate (0.125 mmol) in 1.5 ml of benzene/hexane (2:1) under Ar atmosphere in a screw capped vial. After heating at 80°C for 72 h, the reaction mixture was filtered through a short silica gel column using diethyl ether as an eluent. After evaporation of the solvent, the residue was purified by silica gel column chromatography to afford the corresponding cyclization product.

Conditions C: To $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (10 mol%), PhCOOH (20 mol%) and (*R,R*)-RENORPHOS (60 mol%) was added a substrate (0.125 mmol) in benzene (0.5 M) under Ar atmosphere in a screw capped

vial. After heating at 100°C for 72 h, the reaction mixture was filtered through a short silica gel column using diethyl ether as an eluent. After evaporation of the solvent, the residue was purified by silica gel column chromatography to afford the corresponding cyclization product.

Catalytic Asymmetric Hydroamination of Alkynes

For detail characterization, see our previously reported communications, ref 19 in text.

We have screened several nonracemic chiral ligands for the intramolecular hydroamination reaction, the results are listed below.

Ligand Screened

Entry	L*	Yield (%)	Ee (%)
1	(S)-QUINAP (I)	59	10
2	(R)-BINAP (II)	67	8
3	(R)-MOP (III)	89	6
4	Trost Ligand (1)	51	12
5	(R, R)-Me-BPE (IV)	No Reaction	-
6	(R, R)-Me-DUPHOS (V)	No Reaction	-
7	(S, S)-Me-FerroTane (VI)	57	3
8	(S)-PHANEPHOS (VII)	76	8
9	(S, S)-CHIRAPHOS (2)	92	25
10	(R, R)-NORPHOS (3)	5	98
11	(R, R)-RENORPHOS (4)	54	81
12	(S, S)-BDPP (VIII)	70	15
13	(R)-PROPHOS (IX)	61	0
14	(S, S)-DIOP (X)	92	6
15	(S, S)-BPPM (XI)	81	6
16	(+) NMDPP (XII)	81	5
17	(R)-(S)-JOSIPHOS (XIII)	77	7
18	(R)-(S)-BPPFOAc (XIV)	65	4
19	(XV)	91	0
20	(XVI)	89	0
21	(XVII)	41	6

(S)-QUINAP (I)

(R)-BINAP (II)

(R)-MOP (III)

Trost Ligand (1)

(R, R)-Me-BPE (IV)

(R, R)-Me-DUPHOS (V)

(S, S)-Me-FerroTane (VI)

(S)-PHANEPHOS (VII)

(S, S)-CHIRAPHOS (2)

(R, R)-NORPHOS (3)

(R, R)-RENORPHOS (4)

(S, S)-BDPP (VIII)

(R)-PROPHOS (IX)

(S, S)-DIOP (X)

(S, S)-BPPM (XI)

(+) NMDPP (XII)

(R)-(S)-JOSIPHOS (XIII)

(R)-(S)-BPPFOAc (XIV)

(XV)

(XVI)

(XVII)

Catalytic Asymmetric Hydroalkoxylation of Alkynes

Preparation of Substrates: The substrates were prepared by the Sonogashira reactions of terminal alkynes with corresponding iodo compounds.

General procedure for Sonogashira reaction:

To a mixture of iodobenzenes (1 equiv), Pd(PPh₃)₄ (1 mol%), and CuI (2 mol%) in Et₃N were added alkynes (1 equiv) at room temperature under an argon atmosphere. The mixture was stirred at room temperature overnight. After the reaction was completed, NH₃/NH₄Cl aqueous solution was added and the product was extracted with ether. Then the organic phase was dried with Na₂SO₄ and concentrated. The residue was purified by column chromatography (silica gel, hexane/AcOEt = 4/1) to give corresponding alkynols **7a-i** in high yields.

7a. ¹H NMR (CDCl₃, 400 MHz) δ 7.40-7.37 (m, 2H), 7.29-7.25 (m, 3H), 3.70 (t, *J* = 6.4 Hz, 2H), 2.45 (t, *J* = 6.4 Hz, 2H), 1.77-1.66 (m, 5H); ¹³C NMR (CDCl₃, 100 MHz) δ 131.4, 128.1, 127.5, 123.8, 89.8, 80.9, 62.4, 31.9, 25.0, 19.2; HRMS calcd for C₁₂H₁₄O (M⁺) 174.1045, found 174.1039 (M⁺).

7b. ¹H NMR (CDCl₃, 400 MHz) δ 7.31 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 3.70 (t, *J* = 6.8 Hz, 2H), 2.44 (t, *J* = 6.8 Hz, 2H), 1.75-1.67 (m, 4H), 1.58 (bs, 1H); ¹³C NMR (CDCl₃, 100

MHz)) δ 158.9, 132.7, 115.9, 113.7, 88.2, 80.6, 62.5, 55.3, 32.0, 25.1, 19.2; HRMS calcd for $C_{13}H_{16}O_2$ (M^+) 204.1150, found 227.1043 ($M+Na$).

7c. 1H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 3.71 (t, J = 6.8 Hz, 2H), 2.47 (t, J = 6.8 Hz, 2H), 1.76-1.69 (m, 4H), 1.54 (bs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 131.7, 129.4, 127.7, 125.0, 122.6, 92.7, 79.8, 62.4, 31.9, 24.9, 19.3; HRMS calcd for $C_{13}H_{13}F_3O$ (M^+) 242.0918, found 265.0811 ($M+Na$).

7d. 1H NMR ($CDCl_3$, 400 MHz) δ 7.40-7.36 (m, 2H), 7.29-7.25 (m, 3H), 3.67 (t, J = 6.8 Hz, 2H), 2.42 (t, J = 6.8 Hz, 2H), 1.68-1.50 (m, 6H), 1.48 (bs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 131.4, 128.1, 127.4, 123.9, 90.0, 80.7, 62.8, 32.3, 28.5, 25.1, 19.4; HRMS calcd for $C_{13}H_{16}O$ (M^+) 188.1201, found 211.1093 ($M+Na$).

7e. 1H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 3.67 (t, J = 6.8 Hz, 2H), 2.44 (t, J = 6.8 Hz, 2H), 1.75-1.49 (m, 7H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 131.6, 129.3, 125.3, 124.9, 92.9, 79.6, 62.7, 32.2, 28.4, 25.1, 19.4; HRMS calcd for $C_{14}H_{15}F_3O$ (M^+) 256.1075, found 279.0967 ($M+Na$).

7f. 1H NMR ($CDCl_3$, 400 MHz) δ 7.53-7.26 (m, 9H), 4.79 (s, 2H), 3.88 (s, 2H), 1.50 (bs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.1, 134.9, 131.5, 129.0, 128.3, 128.2, 128.1, 127.8, 127.2, 123.3, 87.3, 82.9, 63.3, 23.1; HRMS calcd for $C_{16}H_{14}O$ (M^+) 222.1045, found 245.0937 ($M+Na$).

7g. 1H NMR ($CDCl_3$, 400 MHz) δ 7.36-7.22 (m, 9H), 4.73 (s, 2H), 2.99 (t, J = 6.8 Hz, 2H), 2.71 (t, J = 6.8 Hz, 2H), 1.99 (bs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.8, 138.4, 131.4, 129.6, 128.5, 128.1, 128.0, 127.6, 126.7, 123.5, 89.4, 81.5, 63.2, 31.4, 21.4; HRMS calcd for $C_{17}H_{16}O$ (M^+) 236.1201, found 259.1093 ($M+Na$).

7h. 1H NMR ($CDCl_3$, 400 MHz) δ 7.51 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 7.37 (d, J = 6.8 Hz, 1H), 7.30-7.24 (m, 3H), 4.77 (s, 2H), 3.03 (t, J = 7.2 Hz, 2H), 2.75 (t, J = 7.2 Hz, 2H), 1.69 (bs, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.7, 138.3, 131.6, 129.7, 129.5, 128.5, 128.1, 127.4, 126.8, 125.2, 125.0, 125.0, 92.2, 80.4, 63.4, 31.2, 21.4; HRMS calcd for $C_{18}H_{15}F_3O$ (M^+) 304.1075, found 304.1070 (M^+).

7i. ^1H NMR (CDCl_3 , 400 MHz) δ 7.37 (d, $J = 6.8$ Hz, 1H), 7.30-7.21 (m, 5H), 6.79 (d, $J = 8.8$ Hz, 2H), 4.77 (s, 2H), 3.79 (s, 3H), 3.01 (t, $J = 7.2$ Hz, 2H), 2.71 (t, $J = 7.2$ Hz, 2H), 1.51 (bs, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 159.0, 138.9, 138.4, 132.8, 129.6, 128.6, 128.0, 126.6, 115.7, 113.8, 87.8, 81.2, 63.3, 55.3, 31.5, 21.5; HRMS calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2$ (M^+) 266.1307, found 289.1301 ($\text{M}+\text{Na}$).

Catalytic Asymmetric Cyclization of alkynols **7**:

The alkynols **7a-i** were subjected to palladium catalysis under condition **C** to give corresponding oxygen heterocycles **8a-i**. Refer Table 3 in the text.

8a. ^1H NMR (CDCl_3 , 400 MHz) δ 7.39-7.20 (m, 5H), 6.58 (d, $J = 16.0$ Hz, 1H), 6.20 (dd, $J = 16.0$, 8.4 Hz, 1H), 4.47 (q, $J = 8.4$ Hz, 1H), 3.97 (q, $J = 8.4$ Hz, 1H), 3.84 (dt, $J = 12.0$, 8.4 Hz, 1H), 2.17-2.09 (m, 1H), 2.01-1.91 (m, 2H), 1.76-1.67 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 136.8, 130.5, 130.3, 128.4, 127.4, 126.4, 79.6, 68.2, 32.4, 25.9; HRMS calcd for $\text{C}_{12}\text{H}_{14}\text{O}$ (M^+) 174.1045, found 174.1039 (M^+); $[\alpha]_{\text{D}}^{23} = -14.1$ (c 0.5, CHCl_3); ee = 80%.

8b. ^1H NMR (CDCl_3 , 400 MHz) δ 7.30 (d, $J = 8.4$ Hz, 2H), 6.82 (d, $J = 8.4$ Hz, 2H), 6.51 (d, $J = 16.0$ Hz, 1H), 6.05 (dd, $J = 16.0$, 6.8 Hz, 1H), 4.43 (q, $J = 7.6$ Hz, 1H), 3.96 (q, $J = 7.6$ Hz, 1H), 3.83 (dt, $J = 12.0$, 7.6 Hz, 1H), 3.79 (s, 3H), 2.16-2.06 (m, 1H), 2.01-1.89 (m, 2H), 1.74-1.65 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 159.0, 130.0, 129.6, 128.2, 127.5, 113.9, 79.9, 68.1, 55.3, 32.5, 25.9; HRMS calcd for $\text{C}_{13}\text{H}_{16}\text{O}_2$ (M^+) 204.1150, found 227.1043 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{15} = -10.8$ (c 1.0, CHCl_3); ee = 40%.

8c. ^1H NMR (CDCl_3 , 400 MHz) δ 7.54 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 6.61 (d, J = 16.0 Hz, 1H), 6.30 (dd, J = 16.0, 6.4 Hz, 1H), 4.49 (q, J = 6.4 Hz, 1H), 3.97 (q, J = 6.4 Hz, 1H), 3.85 (dt, J = 12.0, 6.4 Hz, 1H), 2.19-2.11 (m, 1H), 2.05-1.90 (m, 2H), 1.77-1.67 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 140.3, 133.3, 129.0, 128.7, 126.5, 125.4, 79.2, 68.3, 32.4, 25.9; HRMS calcd for $\text{C}_{13}\text{H}_{13}\text{F}_3\text{O}$ (M^+) 242.0918, found 281.0760 ($\text{M}+\text{O}+\text{Na}$); $[\alpha]_{\text{D}}^{15} = -10.8$ (c 1.0, CHCl_3); ee = 82%.

8d. ^1H NMR (CDCl_3 , 400 MHz) δ 7.31-7.10 (m, 5H), 6.50 (d, J = 16.4 Hz, 1H), 6.13 (dd, J = 16.4, 6.0 Hz, 1H), 4.01-3.98 (m, 1H), 3.92-3.87 (m, 1H), 3.47 (dt, J = 11.6, 2.8 Hz, 1H), 1.90-1.85 (m, 1H), 1.80-1.30 (m, 5H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 136.9, 130.8, 129.7, 128.4, 127.3, 126.3, 78.0, 68.4, 32.3, 25.9, 23.5; HRMS calcd for $\text{C}_{13}\text{H}_{16}\text{O}$ (M^+) 188.1201, found 188.1196 (M^+); $[\alpha]_{\text{D}}^{22} = -13.6$ (c 0.9, CHCl_3); ee = 78%.

8e. ^1H NMR (CDCl_3 , 400 MHz) δ 7.53 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 6.61 (d, J = 16.0 Hz, 1H), 6.29 (d, J = 16.0, 5.6 Hz, 1H), 4.09-4.06 (m, 1H), 4.01-3.97 (m, 1H), 3.58-3.51 (m, 1H), 1.95-1.85 (m, 1H), 1.79-1.71 (m, 1H), 1.66-1.42 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 140.5, 133.4, 129.3, 128.9, 126.4, 125.4, 122.8, 77.6, 68.5, 32.2, 25.9, 23.5; HRMS calcd for $\text{C}_{14}\text{H}_{15}\text{F}_3\text{O}$ (M^+) 256.1075, found 256.1000 (M^+); $[\alpha]_{\text{D}}^{16} = -18.8$ (c 0.9, CHCl_3); ee = 74%.

8f. ^1H NMR (CDCl_3 , 400 MHz) δ 7.42-7.17 (m, 9H), 6.74 (d, J = 16.0 Hz, 1H), 6.28 (dd, J = 16.0, 8.0 Hz, 1H), 5.76 (d, J = 8.0 Hz, 1H), 5.19 (ABq, J = 14.4 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 140.8, 139.1, 136.4, 131.9, 128.9, 128.5, 127.8, 127.7, 127.3, 126.7, 121.9, 121.0, 85.2, 72.8; HRMS calcd for $\text{C}_{16}\text{H}_{14}\text{O}$ (M^+) 222.1045, found 222.1039 (M^+); $[\alpha]_{\text{D}}^{16} = +4.7$ (c 1.1, CHCl_3); ee = 88%.

8g. ^1H NMR (CDCl_3 , 400 MHz) δ 7.41 (d, J = 7.2 Hz, 2H), 7.32 (t, J = 7.2 Hz, 2H), 7.19-7.12 (m, 4H), 7.04-7.01 (m, 1H), 6.71 (d, J = 15.6 Hz, 1H), 6.35 (dd, J = 15.6, 6.0 Hz, 1H), 4.95 (bs, 2H), 4.41-4.36 (m, 1H), 2.93 (dd, J = 16.0, 10.8 Hz, 1H), 2.86 (dd, J = 16.0, 3.6 Hz, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 134.4, 129.4, 128.7, 128.5, 127.6, 126.5, 126.4, 126.1, 124.7, 124.1, 75.1, 68.0, 34.3; HRMS calcd for $\text{C}_{17}\text{H}_{16}\text{O}$ (M^+) 236.1201, found 259.1093 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{15} = -22.4$ (c 0.4, CHCl_3); ee = 86%.

8h. ^1H NMR (CDCl_3 , 400 MHz) δ 7.57 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.25-7.02 (m, 4H), 6.75 (d, J = 16.0 Hz, 1H), 6.44 (dd, J = 16.0 Hz, 5.6 Hz, 1H), 4.94 (ABq, J = 14.8 Hz, 2H), 4.43-4.38 (m, 1H), 3.00-2.84 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 140.1, 134.2, 132.6, 132.0, 129.6,

129.3, 128.7, 128.3, 126.6, 126.5, 126.2, 125.5, 125.4, 124.2, 74.7, 68.1, 34.2; HRMS calcd for $C_{18}H_{15}F_3O$ (M^+) 304.1075, found 304.1071 (M^+); $[\alpha]_D^{25} = -13.2$ (c 1.3, $CHCl_3$); ee = 86%.

8i. 1H NMR ($CDCl_3$, 400 MHz) δ 7.35 (d, J = 8.4 Hz, 2H), 7.19-7.00 (m, 4H), 6.85 (d, J = 8.4 Hz, 2H), 6.65 (d, J = 15.6 Hz, 1H), 6.21 (dd, J = 15.6, 6.0 Hz, 1H), 4.93 (ABq, J = 14.8 Hz, 2H), 4.39-4.32 (m, 1H), 3.81 (s, 3H), 2.95 (dd, J = 16.4, 10.4 Hz, 1H), 2.85 (dd, J = 16.4, 3.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.2, 134.5, 132.9, 130.6, 129.4, 128.8, 127.7, 127.2, 126.4, 126.0, 124.1, 113.9, 75.3, 68.0, 55.3, 34.4; HRMS calcd for $C_{18}H_{18}O_2$ (M^+) 266.1307, found 266.1302 (M^+); $[\alpha]_D^{24} = -16.9$ (c 0.9, $CHCl_3$); ee = 42%.

Hydrogenation of 8a: To a solution of **8a** (100 mg) in methanol (5 mL) was added 10 mol% Pd/C (20 mg) and the mixture was stirred for 12 h at room temperature. The mixture was filtered through celite and washed with ethyl acetate. The combined filtrates were evaporated to give a residue which on column chromatography purification gave **12** (~70 mg, 68%) in pure form.

(S)-12. 1H NMR ($CDCl_3$, 400 MHz) δ 7.29-7.15 (m, 5H), 3.91-3.78 (m, 2H), 3.73 (q, J = 8.0 Hz, 1H), 2.80-2.62 (m, 2H), 2.03-1.72 (m, 5H), 1.52-1.43 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 142.1, 128.3, 128.2, 125.6, 78.6, 67.7, 37.5, 32.7, 31.4, 25.8; HRMS calcd for $C_{12}H_{16}O$ (M^+) 176.1201, found 176.1196 (M^+); $[\alpha]_D^{25} = +2.8$ (c 1.0, $CHCl_3$).

Catalytic Asymmetric Hydrocarbonation of Alkynes

The substrates **9a-h** were prepared by the previously reported procedure, see ref 10a in the text.

9a. ^1H NMR (CDCl_3 , 400 MHz) δ 7.33-7.29 (m, 2H), 7.24-7.19 (m, 3H), 3.68 (t, $J = 6.8$ Hz, 1H), 2.42 (t, $J = 6.8$ Hz, 2H), 2.04 (q, $J = 7.2$ Hz, 2H), 1.80-1.72 (m, 2H), 1.68-1.60 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 131.5, 128.2, 127.7, 123.4, 112.4, 88.4, 81.7, 30.5, 27.3, 25.8, 22.7, 19.0; HRMS calcd for $\text{C}_{15}\text{H}_{14}\text{N}_2$ (M^+) 222.1157, found 245.1155 ($\text{M}+\text{Na}$).

9b. ^1H NMR (CDCl_3 , 400 MHz) δ 7.32 (d, $J = 9.2$ Hz, 2H), 8.00 (d, $J = 9.2$ Hz, 2H), 3.79 (s, 3H), 3.73 (t, $J = 6.8$ Hz, 1H), 2.46 (t, $J = 6.8$ Hz, 2H), 2.08 (q, $J = 7.2$ Hz, 2H), 1.85-1.77 (m, 2H), 1.72-1.65 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 159.1, 132.8, 115.6, 113.8, 112.4, 86.9, 81.4, 55.2, 30.4, 27.4, 25.8, 22.6, 18.9; HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}$ (M^+) 252.1263, found 275.1155 ($\text{M}+\text{Na}$).

9c. ^1H NMR (CDCl_3 , 400 MHz) δ 7.53 (d, $J = 8.0$ Hz, 2H), 7.48 (d, $J = 8.0$ Hz, 2H), 3.76 (t, $J = 6.8$ Hz, 1H), 2.50 (t, $J = 6.8$ Hz, 2H), 2.00 (q, $J = 7.2$ Hz, 2H), 1.86-1.77 (m, 2H), 1.74-1.65 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 131.7, 125.1, 125.1, 125.0, 124.9, 112.4, 91.3, 91.2, 80.4, 30.3, 27.1, 25.7, 22.6, 18.9; HRMS calcd for $\text{C}_{16}\text{H}_{13}\text{F}_3\text{N}_2$ (M^+) 290.1031, found 313.0923 ($\text{M}+\text{Na}$).

9d. ^1H NMR (CDCl_3 , 400 MHz) δ 7.27 (dd, $J = 8.0, 1.2$ Hz, 2H), 7.08 (d, $J = 8.0$ Hz, 2H), 3.70 (t, $J = 7.2$ Hz, 1H), 2.46 (t, $J = 6.8$ Hz, 2H), 2.32 (s, 3H), 2.06 (q, $J = 6.8$ Hz, 2H), 1.83-1.75 (m, 2H), 1.71-1.63 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 137.7, 131.3, 128.9, 120.3, 112.4, 87.7, 81.6, 30.4, 27.3, 25.7, 22.6, 21.4, 18.9; HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2$ (M^+) 236.1313, found 359.1206 ($\text{M}+\text{Na}$).

9e. ^1H NMR (CDCl_3 , 400 MHz) δ 7.33-7.29 (m, 2H), 7.22-7.18 (m, 3H), 3.69 (t, $J = 6.8$ Hz, 1H), 2.42 (t, $J = 6.8$ Hz, 2H), 2.08 (q, $J = 6.8$ Hz, 2H), 1.81-1.73 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 131.3, 128.1, 127.9, 122.9, 112.4, 87.2, 82.2, 29.8, 25.2, 22.2, 18.2; HRMS calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2$ (M^+) 208.1001, found 231.0893 ($\text{M}+\text{Na}$).

9f. ^1H NMR (CDCl_3 , 400 MHz) δ 7.37-7.34 (m, 2H), 7.26-7.21 (m, 3H), 3.65 (t, $J = 6.8$ Hz, 1H), 2.40 (t, $J = 6.8$ Hz, 2H), 2.02-1.96 (m, 2H), 1.63-1.40 (m, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 131.4, 128.1, 127.5, 123.6, 112.5, 89.3, 81.0, 30.6, 28.0, 27.5, 26.1, 22.5, 19.1; HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2$ (M^+) 236.1314, found 259.1312 ($\text{M}+\text{Na}$).

9g. ^1H NMR (CDCl_3 , 400 MHz) δ 7.27 (d, $J = 8.0$ Hz, 2H), 7.08 (d, $J = 8.0$ Hz, 2H), 3.69 (t, $J = 6.8$ Hz, 1H), 2.43 (t, $J = 6.8$ Hz, 2H), 2.33 (s, 3H), 2.03 (q, $J = 6.8$ Hz, 2H), 1.70-1.51 (m, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 137.6, 131.3, 128.9, 120.6, 112.5, 88.5, 81.1, 30.7, 28.1, 27.5, 26.2, 22.6, 21.4, 19.2; HRMS calcd for $\text{C}_{17}\text{H}_{18}\text{N}_2$ (M^+) 250.1470, found 273.1362 ($\text{M}+\text{Na}$).

9h. ^1H NMR (CDCl_3 , 400 MHz) δ 7.51 (d, $J = 8.4$ Hz, 2H), 7.45 (d, $J = 8.4$ Hz, 2H), 3.73 (t, $J = 6.8$ Hz, 1H), 2.43 (t, $J = 6.8$ Hz, 2H), 2.01 (q, $J = 6.8$ Hz, 2H), 1.68-1.40 (m, 6H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 131.6, 127.5, 125.0, 112.5, 92.2, 79.9, 30.6, 27.9, 27.5, 26.1, 22.6, 19.1; HRMS calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_2$ (M^+) 304.1187, found 327.1080 ($\text{M}+\text{Na}$).

Catalytic Asymmetric Cyclization of Alkynylmethines **9a-h**:

The alkynylmethines **9a-h** were subjected to palladium catalysis under condition **A** or **B** to give corresponding carbocycles **10a-h**. Refer Table 4 in the text.

10a. ^1H NMR (CDCl_3 , 400 MHz) δ 7.36-7.17 (m, 5H), 6.63 (d, $J = 16$ Hz, 1H), 6.13 (dd, $J = 16.0$, 8.4 Hz, 1H), 3.06 (q, $J = 8.4$ Hz, 1H), 2.54 (ddd, $J = 13.2$, 8.4, 4.8 Hz, 1H), 2.37-2.29 (m, 1H), 2.14-1.82 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 135.6, 135.5, 128.6, 128.3, 126.6, 123.6, 115.9, 114.4, 54.6, 40.7, 38.3, 30.0, 22.3; HRMS calcd for $\text{C}_{15}\text{H}_{14}\text{N}_2$ (M^+) 222.1157, found 245.1049 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = -155.6$ (c 0.4, CHCl_3); ee = 90%

10b. ^1H NMR (CDCl_3 , 400 MHz) δ 7.35 (d, $J = 8.8$ Hz, 2H), 6.85 (d, $J = 8.8$ Hz, 2H), 6.64 (d, $J = 16.0$ Hz, 1H), 6.06 (dd, $J = 16.0$, 8.8 Hz, 1H), 3.81 (s, 3H), 3.12 (q, $J = 8.8$ Hz, 1H), 2.60 (ddd, $J = 13.2$, 8.8, 4.8 Hz, 1H), 2.44-2.37 (m, 1H), 2.21-1.89 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 159.7, 134.9, 128.5, 127.9, 121.3, 115.9, 114.5, 114.0, 55.3, 54.8, 40.8, 38.3, 30.1, 22.4; HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}$ (M^+) 252.1263, found 275.1155 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = +46.9$ (c 0.4, CHCl_3); ee = 71%

10c. ^1H NMR (CDCl_3 , 400 MHz) δ 7.58 (d, $J = 8.0$ Hz, 2H), 7.50 (d, $J = 8.0$ Hz, 2H), 6.74 (d, $J = 16.0$ Hz, 1H), 6.31 (dd, $J = 16.0$, 8.4 Hz, 1H), 3.17 (q, $J = 8.8$ Hz, 1H), 2.63 (ddd, $J = 13.2$, 8.4, 4.8 Hz, 1H), 2.47-2.39 (m, 1H), 2.25-2.18 (m, 1H), 2.14-1.90 (m, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 139.1, 134.2, 126.5, 125.6, 125.5, 115.7, 114.2, 54.4, 40.6, 38.3, 29.9, 22.4; HRMS calcd for $\text{C}_{16}\text{H}_{13}\text{F}_3\text{N}_2$ (M^+) 290.1031, found 313.0923 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = -31.3$ (c 0.3, CHCl_3); ee = 68%

10d. ^1H NMR (CDCl_3 , 400 MHz) δ 7.30 (d, $J = 8.0$ Hz, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 6.66 (d, $J = 15.6$ Hz, 1H), 6.15 (dd, $J = 15.6$, 8.4 Hz, 1H), 3.14 (q, $J = 8.0$ Hz, 1H), 2.60 (ddd, $J = 13.2$, 8.4, 4.8 Hz, 1H), 2.44-2.38 (m, 1H), 3.34 (s, 3H), 2.21-1.87 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 138.2, 135.4, 132.9, 129.2, 126.5, 122.6, 115.9, 114.4, 54.7, 40.7, 38.3, 30.1, 22.3, 21.3; HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2$ (M^+) 236.1313, found 259.1206 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = +25.4$ (c 0.35, CHCl_3); ee = 88%

10e. ^1H NMR (CDCl_3 , 400 MHz) δ 7.40 (s, 5H), 6.07-6.04 (m, 1H), 5.72 (ddd, $J = 6.8$, 4.8, 2.4 Hz, 1H), 3.93 (t, $J = 2.4$ Hz, 1H), 2.53-2.29 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 136.1, 129.2, 128.9, 128.7, 128.0, 124.9, 115.7, 113.7, 48.0, 38.0, 30.5, 21.5; HRMS calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2$ (M^+) 208.1001, found 231.1001 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = -29.8$ (c 0.32, CHCl_3); determination of ee proved difficult.

10f. ^1H NMR (CDCl_3 , 400 MHz) δ 7.35-7.16 (m, 5H), 6.60 (d, $J = 15.6$ Hz, 1H), 6.10 (dd, $J = 15.6$, 8.8 Hz, 1H), 2.53 (ddd, $J = 11.6$, 8.8, 7.2 Hz, 1H), 2.40 (d, $J = 13.2$ Hz, 1H), 1.93-1.76 (m, 4H), 1.65-1.52

(m, 2H), 1.35-1.28 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 135.8, 134.9, 128.5, 128.1, 126.6, 125.8, 115.9, 113.9, 47.7, 39.0, 35.1, 28.1, 23.9, 21.3; HRMS calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2$ (M^+) 236.1313, found 259.1206 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = -175.4$ (*c* 0.33, CHCl_3); ee = 72%

10g. ^1H NMR (CDCl_3 , 400 MHz) δ 7.30 (d, $J = 8.0$ Hz, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 6.63 (d, $J = 15.6$ Hz, 1H), 6.12 (dd, $J = 15.6, 8.4$ Hz, 1H), 2.58 (dt, $J = 8.4, 3.2$ Hz, 1H), 2.47 (d, $J = 14.0$ Hz, 1H), 2.18 (s, 3H), 1.99-1.85 (m, 4H), 1.70-1.57 (m, 2H), 1.42-1.32 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 138.1, 134.7, 133.0, 129.2, 126.5, 124.7, 115.9, 113.9, 47.7, 39.1, 35.1, 28.2, 23.9, 21.3, 21.2; HRMS calcd for $\text{C}_{17}\text{H}_{18}\text{N}_2$ (M^+) 250.1470, found 273.1362 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = +19.3$ (*c* 0.53, CHCl_3); ee = 76%

10h. ^1H NMR (CDCl_3 , 400 MHz) δ 7.58 (d, $J = 8.4$ Hz, 2H), 7.50 (d, $J = 8.4$ Hz, 2H), 7.00 (d, $J = 15.6$ Hz, 1H), 2.28 (dd, $J = 15.6, 8.8$ Hz, 1H), 2.64 (ddd, $J = 11.2, 8.8, 2.8$ Hz, 1H), 2.50 (d, $J = 13.6$ Hz, 1H), 2.03-1.86 (m, 4H), 1.75-1.60 (m, 2H), 1.45-1.35 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 139.2, 133.6, 128.5, 126.8, 125.6, 125.5, 125.5, 125.4, 125.3, 115.8, 113.8, 47.7, 38.8, 35.0, 27.9, 23.8, 21.2; HRMS calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_2$ (M^+) 304.1187, found 327.1080 ($\text{M}+\text{Na}$); $[\alpha]_{\text{D}}^{25} = +21.3$ (*c* 0.53, CHCl_3); ee = 61%

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4.0993 sec
2.9010 sec
5.50 usec
25.5 g
CD2CL
0.00 ppm
0.30 Hz
9

C:\Documents and Settings\All Users\My Documents\DATA\514\Nmr\Chapter 2\Chapter-5Wp-368 pure Sm.als

C:\Documents and Settings\All Users\My Documents\DATA\514\Nmr\Chapter 2\Chapter-5Wp-368 pure Sm.als
 Wed Jul 21 16:27:02 2004
 1H
 399.65 MHz
 124.00 KHz
 10500.00 Hz
 32768
 7993.60 Hz
 8
 4.0993 sec
 2.9010 sec
 5.50 usec
 1H
 30.5 c
 CDCL3
 0.00 ppm
 0.10 Hz
 9

C:\Documents and Settings\YALI Users\YALI\MyChapter 2\Chapter-5\Np-366 sm.als

DFILE C:\Documents and Settings\YALI Users\YALI
 CONNT Np-366 sm
 DATIM Wed Jul 14 10:15:15 2004
 ORNUC 1H
 EXMOD NON
 OBPRO 399.65 MHz
 OBSET 124.00 MHz
 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 7993.60 Hz
 SCANS 8
 ACQTM 4.0993 sec
 PD 2.9010 sec
 PH 5.50 usec
 TRNUC 1H
 CTEMP 24.5 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BF 0.12 Hz
 RGAIN 11

1.491
1.497
1.502
1.514
1.530
1.539
1.547
1.553
1.574
1.591
1.598
1.607
1.625
1.652
1.680
1.689
1.699
2.001
2.017
2.037
2.404
2.421
3.636
3.642
3.653
3.659
3.670

7.210
7.225
7.234
7.240
7.247
7.252
7.261
7.343
7.344
7.348
7.356
7.364
7.368

Documents and Settings\All Users\Documents\DATA514\Nirmal\chapter 2\Chapter-5\NP-417 pure proton. als

c:\Documents and Settings\All Users\

DFILE
COMMIT
DATE Tue Sep 14 19:32:55 2004
OBNUC 1H
EXNO NON
OBFO 399.65 MHz
OBSE 124.00 KHz
OBFT 10500.00 Hz
POINT 32768
FREQ 7993.60 Hz
SCANS 8
ACQIN 4.0993 sec
PD 2.9010 sec
PMT 5.50 usec
IRNUC 1H
CTEMP 26.3 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 0.30 Hz
RGAIN 10

0.000

3.705
3.687
3.670
3.442
2.426
2.409
2.326
2.310
2.063
2.045
2.025
2.007
1.695
1.674
1.656
1.636
1.619
1.602
1.584
1.567
1.549
1.529

7.284
7.264
7.243
7.092
7.073

6.04

3.01

1.00

1.97

1.86

Y:\Documents and Settings\YALI Users\Documents

Thu Sep 02 17:37:36 2004

DFILE
COMPT
DATIN
DEMIC
EXMCO
CHERO
COSSE
COSSE
POINT
FREOU
SCANS
ACQTN
PD
PMT
IRNUC
CTEMP
SLVMT
EXREF
BF
RGAIN

1.493
1.505
1.527
1.543
1.562
1.582
1.601
1.616
1.634
1.651
1.677
1.685
2.002
2.024
2.041
2.414
2.431
2.448

3.712
3.729
3.746

7.525
7.504
7.469
7.447

399.65 MHz
124.00 KHz
10500.00 Hz
32768
7993.60 Hz
8
4.0953 sec
2.9010 sec
5.50 usec
25.0 c
7.24 ppm
0.50 Hz
6

-337 pure

DFILE
COMMIT
DATIN
OBRUC
EXMOD
OBFRO
OBFET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVMT
EXREF
BF
RGAIN

C:\Documents and Settings\YALI Users\YD
Mp-337 pure
Thu Nov 25 15:52:25 2004
1H
1H
NON

399.65 MHz
124.00 KHz
10500.00 Hz
32768
7993.60 Hz
8
4.0993 sec
2.9010 sec
5.50 usec
21.5 c
0.00 ppm
0.10 Hz
11

C:\Documents and Settings\All Users\Documents\DATA\514\NMR\Chapter 2\Chapter-5\Np-406 after colum (Meo). pure. als

DFILE
C:\Documents and Settings\All Users\Documents\DATA\514\NMR\Chapter 2\Chapter-5\Np-406 after colum (Meo). pure. als
Mod Sep 08 14:43:43 2004
1H
NON
399.65 MHz
124.00 kHz
10500.00 Hz
32768
7993.60 Hz
8
4.0953 sec
2.9010 sec
5.50 usec
26.5 c
CDCl3
0.00 ppm
0.10 Hz
14

Documents and Settings\All Users\Documents\DATA\514\NMR\Chapter 2\Chapter-5\hp-396 pure pd.als

C:\Documents and Settings\All Users\

Sat Aug 28 17:57:51 2004

c:\Documents and Settings\All Users\My Documents\DATA\514\NMR\Chapter 2\Chapter-5\NP-411 after col pure pd.als

c:\Documents and Settings\All Users\My Documents\DATA\514\NMR\Chapter 2\Chapter-5\NP-411 after col pure pd.als

DFIL 0.000
 COMMT 1.893
 DATIM 1.912
 EXMUC 1.919
 EXMUC 1.926
 EXMUC 1.939
 EXMUC 1.943
 EXMUC 1.968
 EXMUC 1.993
 EXMUC 2.002
 EXMUC 2.006
 EXMUC 2.014
 EXMUC 2.018
 EXMUC 2.024
 EXMUC 2.026
 EXMUC 2.036
 EXMUC 2.046
 EXMUC 2.056
 EXMUC 2.076
 EXMUC 2.080
 EXMUC 2.100
 EXMUC 2.136
 EXMUC 2.156
 EXMUC 2.167
 EXMUC 2.177
 EXMUC 2.186
 EXMUC 2.197
 EXMUC 2.341
 EXMUC 2.360
 EXMUC 2.379
 EXMUC 2.384
 EXMUC 2.393
 EXMUC 2.403
 EXMUC 2.413
 EXMUC 2.418
 EXMUC 2.437
 EXMUC 2.568
 EXMUC 2.580
 EXMUC 2.589
 EXMUC 2.601
 EXMUC 2.614
 EXMUC 2.623
 EXMUC 2.635
 EXMUC 3.114
 EXMUC 3.135
 EXMUC 3.140
 EXMUC 6.123
 EXMUC 6.144
 EXMUC 6.162
 EXMUC 6.183
 EXMUC 6.650
 EXMUC 6.689
 EXMUC 7.126
 EXMUC 7.145
 EXMUC 7.239
 EXMUC 7.296
 EXMUC 7.316

399.65 MHz
 124.00 MHz
 10500.00 Hz
 32768
 7993.60 Hz
 4.0993 sec
 2.9010 sec
 5.50 usec
 25.5 c
 0.00 ppm
 0.10 Hz
 11

c:\Documents and Settings\All Users\Documents\DATA\4514\NMR\Chapter 2\Chapter-5\NP-369 Pure proton.als

DFILE	COMMT	DATIM	Sat Jul 24 19:02:07 2004
EXMOD	NON	PROB	1H
NUC1	1H	PROB	1H
NUC2	1H	PROB	1H
NUC3	1H	PROB	1H
NUC4	1H	PROB	1H
NUC5	1H	PROB	1H
NUC6	1H	PROB	1H
NUC7	1H	PROB	1H
NUC8	1H	PROB	1H
NUC9	1H	PROB	1H
NUC10	1H	PROB	1H
NUC11	1H	PROB	1H
NUC12	1H	PROB	1H
NUC13	1H	PROB	1H
NUC14	1H	PROB	1H
NUC15	1H	PROB	1H
NUC16	1H	PROB	1H
NUC17	1H	PROB	1H
NUC18	1H	PROB	1H
NUC19	1H	PROB	1H
NUC20	1H	PROB	1H
NUC21	1H	PROB	1H
NUC22	1H	PROB	1H
NUC23	1H	PROB	1H
NUC24	1H	PROB	1H
NUC25	1H	PROB	1H
NUC26	1H	PROB	1H
NUC27	1H	PROB	1H
NUC28	1H	PROB	1H
NUC29	1H	PROB	1H
NUC30	1H	PROB	1H
NUC31	1H	PROB	1H
NUC32	1H	PROB	1H
NUC33	1H	PROB	1H
NUC34	1H	PROB	1H
NUC35	1H	PROB	1H
NUC36	1H	PROB	1H
NUC37	1H	PROB	1H
NUC38	1H	PROB	1H
NUC39	1H	PROB	1H
NUC40	1H	PROB	1H
NUC41	1H	PROB	1H
NUC42	1H	PROB	1H
NUC43	1H	PROB	1H
NUC44	1H	PROB	1H
NUC45	1H	PROB	1H
NUC46	1H	PROB	1H
NUC47	1H	PROB	1H
NUC48	1H	PROB	1H
NUC49	1H	PROB	1H
NUC50	1H	PROB	1H
NUC51	1H	PROB	1H
NUC52	1H	PROB	1H
NUC53	1H	PROB	1H
NUC54	1H	PROB	1H
NUC55	1H	PROB	1H
NUC56	1H	PROB	1H
NUC57	1H	PROB	1H
NUC58	1H	PROB	1H
NUC59	1H	PROB	1H
NUC60	1H	PROB	1H
NUC61	1H	PROB	1H
NUC62	1H	PROB	1H
NUC63	1H	PROB	1H
NUC64	1H	PROB	1H
NUC65	1H	PROB	1H
NUC66	1H	PROB	1H
NUC67	1H	PROB	1H
NUC68	1H	PROB	1H
NUC69	1H	PROB	1H
NUC70	1H	PROB	1H
NUC71	1H	PROB	1H
NUC72	1H	PROB	1H
NUC73	1H	PROB	1H
NUC74	1H	PROB	1H
NUC75	1H	PROB	1H
NUC76	1H	PROB	1H
NUC77	1H	PROB	1H
NUC78	1H	PROB	1H
NUC79	1H	PROB	1H
NUC80	1H	PROB	1H
NUC81	1H	PROB	1H
NUC82	1H	PROB	1H
NUC83	1H	PROB	1H
NUC84	1H	PROB	1H
NUC85	1H	PROB	1H
NUC86	1H	PROB	1H
NUC87	1H	PROB	1H
NUC88	1H	PROB	1H
NUC89	1H	PROB	1H
NUC90	1H	PROB	1H
NUC91	1H	PROB	1H
NUC92	1H	PROB	1H
NUC93	1H	PROB	1H
NUC94	1H	PROB	1H
NUC95	1H	PROB	1H
NUC96	1H	PROB	1H
NUC97	1H	PROB	1H
NUC98	1H	PROB	1H
NUC99	1H	PROB	1H
NUC100	1H	PROB	1H

c:\Documents and Settings\All Users\Documents\DATA\514\NMR\1Wp-333 after col all the compd.als

DFIL: 1.289
 COM: 1.320
 DAT: 1.502
 CN: 1.551
 EX: 1.557
 MOD: 1.579
 NON: 1.586
 399.65 MHz
 124.00 KHz
 10500.00 Hz
 32768
 POINT
 FREQU 7993.60 Hz
 SCANS 8
 ACQIM 4.0993 sec
 PD 2.9010 sec
 PFI 5.50 usec
 III
 IRNUC 24.0 c
 CTENP
 SLVNT CDCl3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 10

[illegible]

Tue Sep 07 22:51:00 2004

DFILE
CONHT
DATIN
ORNUC
EXMCD
ORFRO
ORSET
ORFIN
POINT
FREQU
SCANS
ACQTM
PD
PMT
IRRUC
CTEMP
SLVNT
EXREF
BF
RGAIN

1H
NON
399.65 MHz
124.00 KHz
10560.00 Hz
32768
7993.60 Hz
8
4.0993 sec
2.9010 sec
5.50 usec
1H
26.1 c
CDCL3
0.00 ppm
0.10 Hz
10

7.593
7.572
7.515
7.494
7.250
6.735
6.696
6.317
6.295
6.277
6.256

C:\Documents and Settings\Wall Users\My

DF11E
COMMIT
DATIM Wed Jun 30 17:27:16 2004

ORNUC 1H
EXMOD NON
ORFREQ 399.65 MHz
ORSET 124.00 KHz
ORF1IN 10500.00 Hz
POINT 32768
FREQU 7993.60 Hz
SCANS 8
ACQIN 4.0993 sec
PD 2.9010 sec
PWI 5.50 usec
IRNUC 1H
CTEMP 25.0 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 17

Cartesian Coordinates

π -Allyl intermediate in hydroamination, isomer I

E(RB+HF-LYP) = -3416.61274125 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.540749	3.444527	2.912290
2	6	0	-3.172421	3.101594	1.525764
3	6	0	-3.450956	1.181603	2.750033
4	6	0	-2.829236	2.165783	3.785165
5	1	0	-1.473358	3.666459	2.847247
6	1	0	-3.031815	4.328824	3.334092
7	1	0	-1.924527	1.765854	4.258194
8	1	0	-3.549224	2.383529	4.582663
9	6	0	-4.354886	2.167552	1.950388
10	1	0	-4.884181	1.716390	1.104534

11	1	0	-5.085261	2.670034	2.593921
12	6	0	-2.352576	2.037105	0.738303
13	1	0	-2.997900	1.737538	-0.100470
14	6	0	-2.290228	0.847537	1.750623
15	1	0	-1.339386	0.879337	2.298839
16	1	0	-3.444225	3.974564	0.926022
17	1	0	-3.941866	0.314513	3.197505
18	15	0	-2.135739	-0.764043	0.752530
19	15	0	-0.679898	2.207176	-0.148245
20	6	0	-0.989198	3.340320	-1.606553
21	6	0	0.016787	4.226250	-2.052327
22	6	0	-2.201561	3.259624	-2.328752
23	6	0	-0.193774	5.029372	-3.188460
24	1	0	0.956758	4.306417	-1.513489
25	6	0	-2.410631	4.065878	-3.462025
26	1	0	-2.991539	2.578026	-2.024126
27	6	0	-1.408299	4.954791	-3.896136
28	1	0	0.586055	5.712751	-3.514569
29	1	0	-3.351939	3.999918	-4.001441
30	1	0	-1.572011	5.579129	-4.770361
31	6	0	0.555803	3.090948	0.935117
32	6	0	1.644248	2.361569	1.456670
33	6	0	0.427344	4.466180	1.238753
34	6	0	2.595743	2.995414	2.278959
35	1	0	1.774570	1.310309	1.219469
36	6	0	1.376796	5.096619	2.061104
37	1	0	-0.399844	5.044948	0.835604
38	6	0	2.461846	4.361992	2.584862
39	1	0	3.433662	2.419417	2.660416
40	1	0	1.271791	6.153373	2.292345
41	1	0	3.195356	4.854342	3.218118
42	6	0	-3.786015	-1.056774	-0.067738
43	6	0	-3.884910	-0.919663	-1.468271
44	6	0	-4.938715	-1.376593	0.684454
45	6	0	-5.124844	-1.089709	-2.112321
46	1	0	-2.995490	-0.698381	-2.053645
47	6	0	-6.175953	-1.548293	0.039278
48	1	0	-4.875645	-1.504129	1.761821
49	6	0	-6.272539	-1.401787	-1.359789
50	1	0	-5.191653	-0.989004	-3.192502
51	1	0	-7.058406	-1.796275	0.623074
52	1	0	-7.230078	-1.537329	-1.855792
53	6	0	-1.923148	-2.137367	1.997652
54	6	0	-1.189660	-1.916824	3.184969
55	6	0	-2.426744	-3.427981	1.724475
56	6	0	-0.979868	-2.968414	4.094839
57	1	0	-0.778504	-0.937250	3.415067
58	6	0	-2.217124	-4.476925	2.638615
59	1	0	-2.981434	-3.620753	0.810585
60	6	0	-1.495156	-4.251488	3.826016
61	1	0	-0.417819	-2.785996	5.006929
62	1	0	-2.616280	-5.464302	2.421765

63	1	0	-1.335000	-5.062743	4.531175
64	46	0	-0.244161	-0.145965	-0.669818
65	6	0	0.569622	-2.182588	-1.304029
66	6	0	1.079596	-1.167537	-2.167181
67	6	0	1.774768	-0.054136	-1.628095
68	1	0	0.788583	-1.148779	-3.216990
69	1	0	2.249478	-0.178394	-0.654719
70	1	0	1.114081	-2.360913	-0.373930
71	6	0	-0.265233	-3.313142	-1.761039
72	6	0	-1.026575	-3.274420	-2.957639
73	6	0	-0.284804	-4.500012	-0.987669
74	6	0	-1.766364	-4.391323	-3.372442
75	1	0	-1.047459	-2.372055	-3.565473
76	6	0	-1.024688	-5.619801	-1.404050
77	1	0	0.295604	-4.547904	-0.068704
78	6	0	-1.767927	-5.571420	-2.598961
79	1	0	-2.341764	-4.347723	-4.293771
80	1	0	-1.014878	-6.526602	-0.804935
81	1	0	-2.338216	-6.437257	-2.925047
82	6	0	2.343103	1.061121	-2.482537
83	1	0	2.405054	1.981052	-1.886875
84	1	0	1.671602	1.269570	-3.326705
85	6	0	3.757561	0.756525	-3.060563
86	1	0	3.715183	-0.135368	-3.703273
87	1	0	4.037158	1.595020	-3.714861
88	6	0	4.904613	0.593738	-2.033369
89	1	0	4.809679	1.332927	-1.229262
90	1	0	5.868461	0.766516	-2.527970
91	7	0	4.964226	-0.749440	-1.411254
92	1	0	4.983231	-1.597045	-1.973999
93	16	0	4.662228	-1.046097	0.263568
94	8	0	4.046281	0.296538	0.919403
95	8	0	3.943521	-2.479588	0.420877
96	6	0	6.533937	-1.230165	1.049184
97	9	0	7.213997	-0.055618	0.805191
98	9	0	6.450987	-1.460810	2.397721
99	9	0	7.165440	-2.278595	0.418749

π -Allyl intermediate in hydroamination, isomer II

E(RB+HF-LYP) = -3416.61177187 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.754269	-2.361009	1.488788
2	6	0	3.555586	-1.783976	2.304409
3	6	0	2.664478	-3.607229	1.235918
4	6	0	4.170606	-3.672951	0.840829
5	1	0	5.130238	-1.660438	0.739322
6	1	0	5.585669	-2.591720	2.164290
7	1	0	4.321060	-3.710387	-0.244618
8	1	0	4.637107	-4.567793	1.269230

9	6	0	2.791676	-3.091329	2.700602
10	1	0	1.835850	-2.905817	3.201580
11	1	0	3.390791	-3.764002	3.323979
12	6	0	2.449715	-1.173669	1.393316
13	1	0	1.589529	-0.993219	2.055661
14	6	0	2.090442	-2.373190	0.457348
15	1	0	2.635510	-2.280312	-0.491203
16	1	0	3.850744	-1.132253	3.130787
17	1	0	2.122103	-4.543899	1.086496
18	15	0	0.282081	-2.158336	-0.086850
19	15	0	2.462077	0.440675	0.389944
20	6	0	2.644927	1.814881	1.640258
21	6	0	3.101009	3.082341	1.215839
22	6	0	2.272943	1.631545	2.990552
23	6	0	3.201372	4.142959	2.132743
24	1	0	3.379329	3.249466	0.179173
25	6	0	2.373472	2.695706	3.905206
26	1	0	1.907856	0.673070	3.347951
27	6	0	2.840771	3.953961	3.480390
28	1	0	3.554139	5.112266	1.791348
29	1	0	2.089695	2.540354	4.942806
30	1	0	2.920291	4.774563	4.188496
31	6	0	3.996188	0.509124	-0.676252
32	6	0	3.887954	0.152577	-2.037703
33	6	0	5.251940	0.893130	-0.156542
34	6	0	5.023674	0.164658	-2.869113
35	1	0	2.919170	-0.121628	-2.450728
36	6	0	6.384407	0.912807	-0.990127
37	1	0	5.349253	1.180964	0.886641
38	6	0	6.274235	0.545047	-2.346594
39	1	0	4.931212	-0.112096	-3.916221
40	1	0	7.346974	1.211696	-0.583702
41	1	0	7.151546	0.561230	-2.987883
42	6	0	-0.791998	-2.456833	1.408802
43	6	0	-1.503389	-1.369046	1.958931
44	6	0	-0.881363	-3.729330	2.017709
45	6	0	-2.293511	-1.548115	3.110319
46	1	0	-1.451655	-0.390226	1.487182
47	6	0	-1.670906	-3.905571	3.167566
48	1	0	-0.350628	-4.579980	1.598290
49	6	0	-2.376016	-2.815061	3.717589
50	1	0	-2.840021	-0.705775	3.525613
51	1	0	-1.736593	-4.886331	3.631088
52	1	0	-2.986651	-2.955270	4.605705
53	6	0	-0.078597	-3.542637	-1.286283
54	6	0	0.897257	-3.922808	-2.235180
55	6	0	-1.343883	-4.169860	-1.308469
56	6	0	0.616808	-4.925673	-3.180258
57	1	0	1.876754	-3.450677	-2.247836
58	6	0	-1.621884	-5.172346	-2.256532
59	1	0	-2.107352	-3.894217	-0.585860
60	6	0	-0.643791	-5.554410	-3.194139

61	1	0	1.378422	-5.215140	-3.899548
62	1	0	-2.596344	-5.653749	-2.258447
63	1	0	-0.858836	-6.331122	-3.923052
64	46	0	0.346541	0.159633	-0.837791
65	6	0	-1.446788	0.230099	-2.163170
66	6	0	-1.175515	1.545547	-1.683916
67	6	0	0.077955	2.162917	-1.948553
68	1	0	-1.857038	1.982163	-0.956875
69	1	0	0.625235	1.828142	-2.834019
70	1	0	-0.935125	-0.086562	-3.078845
71	6	0	-4.534519	1.291241	-2.590890
72	1	0	-5.075816	1.613306	-3.489255
73	1	0	-3.767245	2.048883	-2.392642
74	7	0	-5.563066	1.294092	-1.505191
75	1	0	-6.511840	1.582324	-1.750120
76	6	0	0.473966	3.496120	-1.451882
77	6	0	1.532177	4.176408	-2.104765
78	6	0	-0.193035	4.149477	-0.383661
79	6	0	1.902495	5.475921	-1.720107
80	1	0	2.051124	3.691656	-2.930363
81	6	0	0.175938	5.447491	-0.001320
82	1	0	-1.000600	3.652883	0.148737
83	6	0	1.221478	6.119472	-0.668228
84	1	0	2.705842	5.987619	-2.243845
85	1	0	-0.350336	5.937443	0.813652
86	1	0	1.496117	7.129613	-0.375551
87	6	0	-2.748587	-0.501892	-1.877459
88	1	0	-2.582737	-1.578606	-2.003963
89	1	0	-3.055954	-0.342405	-0.839555
90	6	0	-3.901919	-0.092816	-2.841612
91	1	0	-3.523672	-0.103168	-3.875218
92	1	0	-4.697849	-0.846394	-2.788062
93	16	0	-5.179118	1.856659	0.121619
94	8	0	-3.573339	1.945846	0.259664
95	8	0	-6.161917	3.037635	0.590690
96	6	0	-5.731539	0.222279	1.192597
97	9	0	-5.468578	0.437400	2.525466
98	9	0	-7.076903	0.008343	1.000783
99	9	0	-5.015867	-0.872568	0.750112

π -Allyl intermediate in hydroamination, isomer III

E(RB+HF-LYP) = -3416.61386442 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.607910	3.866803	0.633044
2	6	0	-2.718351	3.166879	1.707188
3	6	0	-1.203266	4.187143	0.320191
4	6	0	-2.573775	4.658554	-0.253062
5	1	0	-4.198054	3.156984	0.048358
6	1	0	-4.311566	4.549649	1.122274
7	1	0	-2.683589	4.441526	-1.322494
8	1	0	-2.688143	5.741117	-0.122871
9	6	0	-1.535955	4.183229	1.842496
10	1	0	-0.722417	3.828560	2.483550
11	1	0	-1.857729	5.169126	2.195843
12	6	0	-1.893291	1.981713	1.123572
13	1	0	-1.168690	1.715090	1.907661

14	6	0	-1.109357	2.664303	-0.044430
15	1	0	-1.641235	2.503149	-0.991490
16	1	0	-3.245798	2.920009	2.632364
17	1	0	-0.352038	4.793995	0.003288
18	15	0	0.508796	1.698384	-0.296863
19	15	0	-2.477797	0.263095	0.568009
20	6	0	-3.157036	-0.577091	2.089645
21	6	0	-4.022596	-1.684438	1.942760
22	6	0	-2.766784	-0.172734	3.385534
23	6	0	-4.502872	-2.363414	3.076698
24	1	0	-4.328993	-2.017991	0.955359
25	6	0	-3.246872	-0.856715	4.517429
26	1	0	-2.097578	0.670025	3.532173
27	6	0	-4.117916	-1.952593	4.367436
28	1	0	-5.173466	-3.209170	2.949801
29	1	0	-2.943848	-0.532144	5.509415
30	1	0	-4.491232	-2.477428	5.242799
31	6	0	-3.919248	0.459400	-0.605569
32	6	0	-3.661504	0.456166	-1.993157
33	6	0	-5.241443	0.640263	-0.144217
34	6	0	-4.710509	0.646912	-2.911620
35	1	0	-2.647449	0.296546	-2.354543
36	6	0	-6.290543	0.819361	-1.063650
37	1	0	-5.456999	0.640824	0.920686
38	6	0	-6.027540	0.828014	-2.448443
39	1	0	-4.502823	0.646752	-3.978700
40	1	0	-7.306158	0.955566	-0.701596
41	1	0	-6.840414	0.969804	-3.155846
42	6	0	1.545280	2.008913	1.224411
43	6	0	1.730186	0.968829	2.158137
44	6	0	2.114974	3.278681	1.469435
45	6	0	2.470904	1.196347	3.333376
46	1	0	1.330599	-0.023048	1.963646
47	6	0	2.854122	3.503257	2.643455
48	1	0	2.000430	4.083480	0.748171
49	6	0	3.030220	2.463718	3.580007
50	1	0	2.619380	0.384232	4.039591
51	1	0	3.293444	4.480647	2.824869
52	1	0	3.607022	2.639054	4.484469
53	6	0	1.412459	2.527472	-1.702733
54	6	0	0.704146	3.199389	-2.723180
55	6	0	2.821009	2.437003	-1.775002
56	6	0	1.397224	3.787341	-3.797276
57	1	0	-0.379127	3.282820	-2.690043
58	6	0	3.508983	3.029823	-2.849808
59	1	0	3.381862	1.915669	-1.003438
60	6	0	2.801734	3.705951	-3.862998
61	1	0	0.843788	4.310494	-4.572807
62	1	0	4.593189	2.965036	-2.890934
63	1	0	3.336684	4.166175	-4.689634
64	46	0	-0.419126	-0.559325	-0.496602
65	6	0	-0.798445	-2.827931	-0.638501

66	6	0	0.052381	-2.395557	-1.691622
67	6	0	1.267556	-1.704437	-1.418301
68	1	0	-0.304612	-2.440137	-2.720120
69	1	0	1.759876	-1.916690	-0.466540
70	1	0	-0.332734	-3.020267	0.331692
71	6	0	-2.099946	-3.496580	-0.842596
72	6	0	-2.880287	-3.321133	-2.014002
73	6	0	-2.570408	-4.385704	0.155106
74	6	0	-4.079361	-4.027290	-2.187099
75	1	0	-2.560033	-2.625816	-2.786468
76	6	0	-3.769751	-5.097046	-0.019954
77	1	0	-1.985997	-4.529799	1.061769
78	6	0	-4.528841	-4.922404	-1.193112
79	1	0	-4.666273	-3.882515	-3.090353
80	1	0	-4.105917	-5.787419	0.749244
81	1	0	-5.455209	-5.473223	-1.332890
82	6	0	2.140920	-1.195063	-2.554167
83	1	0	2.652136	-0.273176	-2.257691
84	1	0	1.495135	-0.935210	-3.403631
85	6	0	3.205134	-2.224242	-3.052122
86	1	0	2.791610	-3.242917	-3.020952
87	1	0	3.421383	-2.011913	-4.109506
88	6	0	4.569687	-2.188728	-2.329099
89	1	0	4.989797	-1.177475	-2.365712
90	1	0	5.279021	-2.856592	-2.834154
91	7	0	4.545098	-2.610758	-0.908680
92	1	0	4.227776	-3.541014	-0.641678
93	16	0	4.448562	-1.461521	0.389644
94	8	0	3.340616	-1.953480	1.457516
95	8	0	4.445186	0.021440	-0.241131
96	6	0	6.250213	-1.693479	1.304745
97	9	0	6.282046	-0.941122	2.450944
98	9	0	6.406856	-3.029240	1.605225
99	9	0	7.233404	-1.285524	0.434415

π -Allyl intermediate in hydroamination, isomer IV

E(RB+HF-LYP) = -3416.61398952 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.700219	-2.073627	3.022215
2	6	0	4.167832	-1.649591	1.595574
3	6	0	3.658517	0.339012	2.619232
4	6	0	3.451205	-0.703848	3.758891
5	1	0	2.806239	-2.701333	3.003875
6	1	0	4.491549	-2.648651	3.516234
7	1	0	2.454157	-0.645720	4.211711
8	1	0	4.185362	-0.544879	4.557364
9	6	0	4.885477	-0.291158	1.895238
10	1	0	5.204509	0.245879	0.995663
11	1	0	5.746781	-0.402088	2.562974
12	6	0	3.009893	-1.071753	0.730177

13	1	0	3.493253	-0.639643	-0.159280
14	6	0	2.477001	0.099508	1.616273
15	1	0	1.601033	-0.242286	2.182810
16	1	0	4.766212	-2.403849	1.077604
17	1	0	3.771051	1.368282	2.967147
18	15	0	1.745946	1.426367	0.470334
19	15	0	1.527753	-1.955062	-0.066569
20	6	0	2.233897	-3.267359	-1.192076
21	6	0	1.479625	-4.420760	-1.504575
22	6	0	3.492876	-3.083065	-1.805999
23	6	0	1.981606	-5.377681	-2.405323
24	1	0	0.513869	-4.588519	-1.034690
25	6	0	3.992106	-4.040597	-2.707550
26	1	0	4.096755	-2.205658	-1.590475
27	6	0	3.239096	-5.191127	-3.010802
28	1	0	1.395268	-6.265173	-2.628897
29	1	0	4.965282	-3.889446	-3.167218
30	1	0	3.627491	-5.931653	-3.704708
31	6	0	3.196535	2.307166	-0.315258
32	6	0	3.577558	1.960985	-1.629795
33	6	0	3.940809	3.277680	0.390838
34	6	0	4.694851	2.570177	-2.230821
35	1	0	2.998866	1.226849	-2.187165
36	6	0	5.054447	3.889166	-0.212700
37	1	0	3.650022	3.568434	1.396607
38	6	0	5.435998	3.535166	-1.522516
39	1	0	4.979411	2.299737	-3.244498
40	1	0	5.620161	4.638024	0.335266
41	1	0	6.295941	4.011162	-1.986344
42	6	0	0.944346	2.682395	1.593681
43	6	0	0.597053	2.362758	2.924720
44	6	0	0.634680	3.963596	1.086156
45	6	0	-0.038744	3.316646	3.740415
46	1	0	0.819116	1.386042	3.343969
47	6	0	0.002150	4.914881	1.905056
48	1	0	0.882521	4.226427	0.061651
49	6	0	-0.336182	4.596012	3.234190
50	1	0	-0.296717	3.060895	4.764765
51	1	0	-0.229565	5.896676	1.501586
52	1	0	-0.825365	5.332762	3.865925
53	46	0	0.435180	0.009252	-1.059650
54	6	0	-0.768912	-0.884196	-2.738401
55	6	0	-1.341579	0.363291	-2.363817
56	6	0	-0.563019	1.552304	-2.446538
57	1	0	-2.295982	0.394726	-1.844825
58	1	0	0.265831	1.553176	-3.159447
59	1	0	0.043504	-0.853525	-3.471818
60	6	0	-1.494078	-2.222900	-2.704444
61	1	0	-1.979906	-2.373089	-3.684896
62	1	0	-0.735445	-3.011987	-2.639785
63	6	0	-2.535243	-2.424423	-1.575323
64	1	0	-2.588111	-3.492238	-1.320323

65	1	0	-2.189343	-1.905367	-0.673658
66	6	0	-3.960344	-1.942494	-1.932904
67	1	0	-3.961372	-0.925683	-2.333908
68	1	0	-4.417352	-2.587549	-2.694719
69	7	0	-4.915449	-1.975041	-0.790301
70	1	0	-5.055823	-2.881606	-0.332672
71	6	0	-1.036015	2.896564	-2.061723
72	6	0	-2.162145	3.108326	-1.224966
73	6	0	-0.364358	4.024956	-2.596670
74	6	0	-2.609575	4.410827	-0.957576
75	1	0	-2.691093	2.268332	-0.782009
76	6	0	-0.812222	5.328125	-2.324189
77	1	0	0.498653	3.877648	-3.244198
78	6	0	-1.942146	5.525797	-1.505809
79	1	0	-3.478204	4.558563	-0.321337
80	1	0	-0.294413	6.180680	-2.755875
81	1	0	-2.300573	6.531792	-1.302749
82	6	0	0.540440	-2.850724	1.243551
83	6	0	-0.631699	-2.233646	1.732348
84	6	0	0.931770	-4.106582	1.759605
85	6	0	-1.409584	-2.859817	2.724848
86	1	0	-0.947368	-1.271334	1.334837
87	6	0	0.156448	-4.730746	2.753323
88	1	0	1.827782	-4.599619	1.392175
89	6	0	-1.013032	-4.109177	3.238285
90	1	0	-2.319852	-2.378574	3.070430
91	1	0	0.463643	-5.695925	3.147580
92	1	0	-1.610519	-4.598125	4.003360
93	16	0	-4.686224	-0.724095	0.467313
94	8	0	-3.819948	0.477270	-0.178753
95	8	0	-4.312460	-1.356779	1.901416
96	6	0	-6.592081	-0.052689	0.594602
97	9	0	-6.936015	0.516312	-0.606218
98	9	0	-7.407137	-1.126410	0.870074
99	9	0	-6.669838	0.875085	1.602424

π -Allyl intermediate in hydroalkoxylation, isomer I

E(RB+HF-LYP) = -2551.06544537 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.870321	-4.277842	-0.544978
2	6	0	1.366085	-3.634345	0.783957
3	6	0	-0.536259	-3.844240	-0.480939
4	6	0	0.551464	-4.513797	-1.373224
5	1	0	2.583444	-3.644828	-1.077513
6	1	0	2.374808	-5.226368	-0.328683
7	1	0	0.602398	-4.077082	-2.377862
8	1	0	0.342520	-5.583723	-1.489565
9	6	0	-0.046372	-4.293952	0.927971
10	1	0	-0.635257	-3.895024	1.760322
11	1	0	-0.000742	-5.384678	1.020383

12	6	0	0.879894	-2.166831	0.597497
13	1	0	0.375118	-1.907089	1.540113
14	6	0	-0.212647	-2.310709	-0.511492
15	1	0	0.220521	-2.064140	-1.489992
16	1	0	2.044008	-3.764601	1.631857
17	1	0	-1.561274	-4.107416	-0.751459
18	15	0	-1.489903	-0.926291	-0.250619
19	15	0	1.884635	-0.580849	0.291587
20	6	0	2.987616	-0.379160	1.787328
21	6	0	4.246169	0.252332	1.671020
22	6	0	2.537619	-0.782617	3.064689
23	6	0	5.045773	0.461624	2.809470
24	1	0	4.615019	0.568554	0.699014
25	6	0	3.339077	-0.572519	4.201192
26	1	0	1.570528	-1.261741	3.191973
27	6	0	4.596480	0.049583	4.078354
28	1	0	6.015327	0.941423	2.703773
29	1	0	2.983495	-0.895426	5.176170
30	1	0	5.216039	0.208695	4.956788
31	6	0	3.021742	-0.820350	-1.170832
32	6	0	2.665480	-0.222934	-2.398603
33	6	0	4.206090	-1.587329	-1.089227
34	6	0	3.473631	-0.400571	-3.537409
35	1	0	1.769482	0.390030	-2.463404
36	6	0	5.016942	-1.756559	-2.225310
37	1	0	4.500554	-2.048270	-0.150078
38	6	0	4.650550	-1.167577	-3.453096
39	1	0	3.189050	0.062222	-4.478703
40	1	0	5.926384	-2.347338	-2.154627
41	1	0	5.278505	-1.302680	-4.329853
42	6	0	-2.474118	-1.393632	1.266958
43	6	0	-2.222938	-0.714611	2.477957
44	6	0	-3.426934	-2.436246	1.237299
45	6	0	-2.906891	-1.080834	3.652337
46	1	0	-1.508024	0.104948	2.499814
47	6	0	-4.112300	-2.798018	2.410479
48	1	0	-3.645803	-2.955364	0.307968
49	6	0	-3.851129	-2.124251	3.621081
50	1	0	-2.710889	-0.550366	4.580614
51	1	0	-4.845814	-3.599363	2.380780
52	1	0	-4.383369	-2.405816	4.525924
53	6	0	-2.684218	-1.039460	-1.680511
54	6	0	-2.282959	-1.574557	-2.924593
55	6	0	-3.991060	-0.521154	-1.539650
56	6	0	-3.180607	-1.604118	-4.007643
57	1	0	-1.283310	-1.976999	-3.063663
58	6	0	-4.886732	-0.555449	-2.623597
59	1	0	-4.317215	-0.099326	-0.593033
60	6	0	-4.485610	-1.096156	-3.860536
61	1	0	-2.863078	-2.025401	-4.957922
62	1	0	-5.892505	-0.162510	-2.500180
63	1	0	-5.179757	-1.123777	-4.696307

64	46	0	0.023870	0.993130	-0.038333
65	6	0	-1.347568	2.771446	-0.402616
66	6	0	-0.177724	3.198207	0.293451
67	6	0	1.111388	2.957990	-0.246390
68	1	0	-0.260626	3.554709	1.319597
69	1	0	1.221760	2.896626	-1.330326
70	1	0	-1.282913	2.716139	-1.491977
71	6	0	-2.720769	2.907578	0.129377
72	6	0	-2.999437	3.010235	1.516481
73	6	0	-3.803896	2.974705	-0.781273
74	6	0	-4.313136	3.191682	1.972469
75	1	0	-2.192163	2.946375	2.242826
76	6	0	-5.120562	3.158039	-0.325156
77	1	0	-3.609531	2.899244	-1.849367
78	6	0	-5.381403	3.268729	1.054211
79	1	0	-4.509151	3.272539	3.038613
80	1	0	-5.936300	3.223669	-1.040519
81	1	0	-6.398035	3.414518	1.409675
82	6	0	2.372920	3.372861	0.484579
83	1	0	3.163750	2.627529	0.333517
84	1	0	2.180950	3.419487	1.565339
85	6	0	2.899523	4.755146	-0.002800
86	1	0	2.064222	5.461067	-0.101429
87	1	0	3.578832	5.161404	0.760311
88	6	0	3.674624	4.702607	-1.322672
89	1	0	4.563299	4.060134	-1.216582
90	1	0	4.001674	5.716021	-1.598685
91	8	0	2.792436	4.154075	-2.365632
92	1	0	3.186886	4.276861	-3.253426

π -Allyl intermediate in hydroalkoxylation, isomer II

E(RB+HF-LYP) = -2551.06430792 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.504416	-3.910438	0.992506
2	6	0	2.066722	-2.745574	1.933819
3	6	0	0.084000	-3.685393	1.265295
4	6	0	1.149224	-4.619258	0.616155
5	1	0	3.045659	-3.560304	0.110696
6	1	0	3.169582	-4.593270	1.533072
7	1	0	1.015594	-4.723745	-0.467180
8	1	0	1.092787	-5.623110	1.053176
9	6	0	0.795425	-3.357833	2.612052
10	1	0	0.254043	-2.651319	3.249878
11	1	0	1.013765	-4.260247	3.193656
12	6	0	1.346618	-1.593242	1.172083
13	1	0	0.921008	-0.947733	1.955364

14	6	0	0.169737	-2.340241	0.464751
15	1	0	0.451508	-2.570706	-0.571114
16	1	0	2.850916	-2.397517	2.611528
17	1	0	-0.914325	-4.123803	1.329890
18	15	0	-1.264084	-1.109604	0.246885
19	15	0	2.059941	-0.286954	-0.011806
20	6	0	3.344036	0.650558	0.971336
21	6	0	4.449242	1.242981	0.320549
22	6	0	3.180800	0.843264	2.361265
23	6	0	5.382600	2.001272	1.050445
24	1	0	4.597041	1.105849	-0.747383
25	6	0	4.114955	1.602622	3.089004
26	1	0	2.337100	0.408693	2.890648
27	6	0	5.219823	2.183630	2.437268
28	1	0	6.234032	2.442242	0.538474
29	1	0	3.981225	1.735961	4.159351
30	1	0	5.943644	2.765573	3.001502
31	6	0	2.992096	-1.130574	-1.396091
32	6	0	2.369318	-1.232573	-2.658611
33	6	0	4.282805	-1.675889	-1.213818
34	6	0	3.021476	-1.880322	-3.724921
35	1	0	1.383429	-0.798593	-2.812152
36	6	0	4.936300	-2.316446	-2.281411
37	1	0	4.780820	-1.601093	-0.250866
38	6	0	4.306337	-2.423515	-3.538248
39	1	0	2.533208	-1.952960	-4.693215
40	1	0	5.929598	-2.731708	-2.133079
41	1	0	4.814261	-2.919378	-4.361175
42	6	0	-1.990614	-0.836671	1.945663
43	6	0	-1.752098	0.393376	2.594645
44	6	0	-2.732223	-1.841024	2.607281
45	6	0	-2.239816	0.615887	3.896125
46	1	0	-1.200200	1.177589	2.081179
47	6	0	-3.221418	-1.615780	3.906023
48	1	0	-2.941000	-2.787064	2.114894
49	6	0	-2.973198	-0.388776	4.554772
50	1	0	-2.055593	1.567972	4.387102
51	1	0	-3.793318	-2.391341	4.408550
52	1	0	-3.353985	-0.217390	5.558253
53	6	0	-2.570518	-2.016804	-0.730541
54	6	0	-2.209980	-2.994136	-1.685140
55	6	0	-3.932238	-1.680224	-0.566825
56	6	0	-3.198969	-3.638401	-2.450206
57	1	0	-1.170020	-3.270251	-1.838089
58	6	0	-4.919080	-2.328799	-1.331543
59	1	0	-4.228785	-0.923079	0.153325
60	6	0	-4.557255	-3.310080	-2.273960
61	1	0	-2.910129	-4.395101	-3.174998
62	1	0	-5.964316	-2.067177	-1.189413
63	1	0	-5.321090	-3.812593	-2.861462
64	46	0	-0.041230	0.795796	-0.702777
65	6	0	-1.705191	1.982742	-1.722158

66	6	0	-0.610711	2.843908	-1.426881
67	6	0	0.690050	2.546201	-1.911491
68	1	0	-0.713536	3.650567	-0.704667
69	1	0	0.767272	1.978582	-2.845108
70	1	0	-1.658364	1.395065	-2.643269
71	6	0	-3.068541	2.179444	-1.184919
72	6	0	-3.328102	2.959719	-0.028331
73	6	0	-4.165614	1.601249	-1.869162
74	6	0	-4.642499	3.162756	0.415731
75	1	0	-2.505859	3.412180	0.520652
76	6	0	-5.483191	1.807673	-1.425787
77	1	0	-3.985084	1.000444	-2.758462
78	6	0	-5.727876	2.590035	-0.281079
79	1	0	-4.826507	3.766976	1.300527
80	1	0	-6.312901	1.368360	-1.973588
81	1	0	-6.745865	2.754846	0.062293
82	6	0	1.920625	3.386594	-1.602793
83	1	0	1.989734	4.173241	-2.374702
84	1	0	2.801437	2.750802	-1.761184
85	6	0	2.034384	4.045561	-0.200666
86	1	0	1.587574	3.399229	0.566123
87	1	0	3.102384	4.118294	0.046143
88	6	0	1.463781	5.460938	-0.048605
89	1	0	1.774898	6.093025	-0.895118
90	1	0	1.846019	5.905658	0.882171
91	8	0	-0.004823	5.396044	0.016667
92	1	0	-0.394166	6.291220	0.094463

π -Allyl intermediate in hydrocarbonation, isomer I

E(RB+HF-LYP) = -2699.57762784 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.515349	-4.580732	-1.666712
2	6	0	-0.959632	-4.135069	-0.237646
3	6	0	-2.444490	-3.079513	-1.632136
4	6	0	-1.600579	-3.944881	-2.614662
5	1	0	0.494980	-4.250023	-1.916356
6	1	0	-0.525589	-5.674479	-1.733493
7	1	0	-1.158008	-3.354101	-3.425355
8	1	0	-2.227344	-4.717825	-3.074387
9	6	0	-2.512890	-4.046403	-0.411846
10	1	0	-3.031422	-3.639773	0.462618
11	1	0	-2.968022	-5.007762	-0.673834
12	6	0	-0.703755	-2.620968	0.025533

13	1	0	-1.239153	-2.393686	0.958843
14	6	0	-1.479064	-1.942783	-1.150059
15	1	0	-0.782719	-1.706687	-1.965538
16	1	0	-0.604997	-4.784081	0.567682
17	1	0	-3.396574	-2.736625	-2.043499
18	15	0	-2.032971	-0.222349	-0.560191
19	15	0	0.932095	-1.702173	0.324065
20	6	0	1.571217	-2.318608	1.973125
21	6	0	2.961410	-2.357520	2.222990
22	6	0	0.677627	-2.675915	3.007944
23	6	0	3.448274	-2.760917	3.479767
24	1	0	3.667604	-2.092460	1.440779
25	6	0	1.167260	-3.079917	4.263468
26	1	0	-0.397948	-2.651828	2.854457
27	6	0	2.553807	-3.124504	4.504463
28	1	0	4.520525	-2.795813	3.654315
29	1	0	0.468410	-3.361628	5.046775
30	1	0	2.930555	-3.440698	5.473458
31	6	0	2.211272	-2.212470	-0.933542
32	6	0	2.604377	-1.283723	-1.918653
33	6	0	2.794153	-3.500818	-0.915512
34	6	0	3.566532	-1.636282	-2.884462
35	1	0	2.192166	-0.279137	-1.928891
36	6	0	3.751358	-3.852273	-1.882405
37	1	0	2.513384	-4.223117	-0.153135
38	6	0	4.136978	-2.922100	-2.871200
39	1	0	3.871430	-0.901362	-3.623338
40	1	0	4.195408	-4.844075	-1.864638
41	1	0	4.880823	-3.196814	-3.614485
42	6	0	-3.406404	-0.487269	0.675510
43	6	0	-3.155593	-0.233973	2.040524
44	6	0	-4.673337	-0.970888	0.277918
45	6	0	-4.155152	-0.473054	3.002270
46	1	0	-2.191474	0.163048	2.349542
47	6	0	-5.671317	-1.206277	1.239642
48	1	0	-4.890304	-1.151992	-0.771357
49	6	0	-5.413428	-0.961837	2.604117
50	1	0	-3.955750	-0.270693	4.051383
51	1	0	-6.643989	-1.576645	0.927067
52	1	0	-6.187772	-1.143540	3.344780
53	6	0	-2.813369	0.614587	-2.034534
54	6	0	-2.316217	0.379780	-3.336220
55	6	0	-3.861718	1.542842	-1.850953
56	6	0	-2.874051	1.049328	-4.440124
57	1	0	-1.502405	-0.320153	-3.506775
58	6	0	-4.419098	2.208640	-2.958145
59	1	0	-4.249419	1.745381	-0.856697
60	6	0	-3.929353	1.963859	-4.255239
61	1	0	-2.488281	0.855473	-5.437463
62	1	0	-5.232842	2.912867	-2.806023
63	1	0	-4.362908	2.476739	-5.109628
64	46	0	0.108355	0.612265	0.279985

65	6	0	-0.261185	2.860637	0.350567
66	6	0	0.860862	2.525541	1.165961
67	6	0	1.969428	1.830551	0.615122
68	1	0	0.796900	2.642643	2.247231
69	1	0	2.153562	1.948980	-0.453875
70	1	0	-0.074575	3.015218	-0.714993
71	6	0	-1.493700	3.498853	0.859756
72	6	0	-1.880021	3.444629	2.223745
73	6	0	-2.309194	4.225366	-0.042724
74	6	0	-3.031199	4.109856	2.669556
75	1	0	-1.284851	2.882950	2.940613
76	6	0	-3.462504	4.892593	0.403735
77	1	0	-2.029192	4.278655	-1.092945
78	6	0	-3.828132	4.839549	1.762453
79	1	0	-3.310524	4.063775	3.719061
80	1	0	-4.067104	5.457246	-0.301168
81	1	0	-4.716807	5.358808	2.111267
82	6	0	3.164495	1.418804	1.456115
83	1	0	3.690883	0.588535	0.968570
84	1	0	2.804941	1.036771	2.420323
85	6	0	4.185334	2.572336	1.749627
86	1	0	3.658254	3.537482	1.783419
87	1	0	4.573608	2.408092	2.763799
88	6	0	5.434429	2.687125	0.840069
89	1	0	5.895861	1.703161	0.690726
90	1	0	6.174922	3.309367	1.357911
91	6	0	5.219539	3.365160	-0.562327
92	1	0	4.624231	4.279294	-0.417650
93	6	0	4.492148	2.500608	-1.518728
94	6	0	6.518300	3.766883	-1.150216
95	7	0	7.563397	4.094504	-1.586250
96	7	0	3.898305	1.794232	-2.251197

π -Allyl intermediate in hydrocarbonation, isomer II

E(RB+HF-LYP) = -2699.57613045 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.074103	-3.671104	1.479117
2	6	0	2.531601	-2.407800	2.217253
3	6	0	0.652623	-3.661228	1.822653
4	6	0	1.799756	-4.580153	1.304825
5	1	0	3.543495	-3.431414	0.522013
6	1	0	3.830572	-4.166340	2.098092
7	1	0	1.649995	-4.900052	0.266758
8	1	0	1.870642	-5.484119	1.920961
9	6	0	1.356644	-3.016326	3.053496

10	1	0	0.754952	-2.266515	3.577802
11	1	0	1.691867	-3.767032	3.777507
12	6	0	1.664580	-1.496827	1.296686
13	1	0	1.188389	-0.766864	1.969587
14	6	0	0.564838	-2.485134	0.790520
15	1	0	0.849970	-2.870981	-0.197065
16	1	0	3.290653	-1.863431	2.785031
17	1	0	-0.288756	-4.182184	2.010202
18	15	0	-1.004241	-1.487322	0.408126
19	15	0	2.185215	-0.360794	-0.138432
20	6	0	3.490794	0.782626	0.550560
21	6	0	4.421120	1.395280	-0.318896
22	6	0	3.518008	1.102354	1.925808
23	6	0	5.370944	2.303671	0.182637
24	1	0	4.419081	1.160062	-1.380316
25	6	0	4.468567	2.011788	2.425291
26	1	0	2.810034	0.654039	2.617117
27	6	0	5.398482	2.615083	1.556526
28	1	0	6.087732	2.760694	-0.494567
29	1	0	4.485113	2.241985	3.487347
30	1	0	6.136769	3.311896	1.944281
31	6	0	3.044494	-1.359827	-1.466137
32	6	0	2.313144	-1.711014	-2.621500
33	6	0	4.390339	-1.772572	-1.344819
34	6	0	2.913668	-2.475487	-3.639431
35	1	0	1.283142	-1.378001	-2.733194
36	6	0	4.990921	-2.530890	-2.365539
37	1	0	4.973191	-1.501098	-0.468706
38	6	0	4.253553	-2.887304	-3.513047
39	1	0	2.342936	-2.738542	-4.526192
40	1	0	6.027198	-2.842589	-2.265598
41	1	0	4.721311	-3.472368	-4.300392
42	6	0	-1.740631	-0.939972	2.034575
43	6	0	-1.691253	0.430193	2.367881
44	6	0	-2.331255	-1.854028	2.936048
45	6	0	-2.222541	0.891243	3.586429
46	1	0	-1.256269	1.144898	1.674554
47	6	0	-2.855755	-1.395050	4.157584
48	1	0	-2.400127	-2.910036	2.687555
49	6	0	-2.801266	-0.023997	4.485527
50	1	0	-2.191725	1.953616	3.809997
51	1	0	-3.309741	-2.101738	4.847409
52	1	0	-3.215956	0.324823	5.427861
53	6	0	-2.214284	-2.703338	-0.326301
54	6	0	-1.760738	-3.821767	-1.061243
55	6	0	-3.602064	-2.473821	-0.201553
56	6	0	-2.683045	-4.707677	-1.646795
57	1	0	-0.699023	-4.021555	-1.178956
58	6	0	-4.521211	-3.363873	-0.786153
59	1	0	-3.970702	-1.613014	0.349497
60	6	0	-4.066577	-4.483176	-1.508754
61	1	0	-2.322572	-5.569516	-2.202384

62	1	0	-5.586693	-3.179911	-0.677370
63	1	0	-4.778705	-5.170889	-1.957158
64	46	0	-0.048512	0.411454	-0.827685
65	6	0	-1.891538	1.221408	-1.967272
66	6	0	-1.015664	2.273862	-1.596136
67	6	0	0.349843	2.272659	-2.006387
68	1	0	-1.354936	3.001229	-0.864113
69	1	0	0.581344	1.786678	-2.958291
70	1	0	-1.638193	0.656751	-2.868621
71	6	0	-3.304009	1.113880	-1.553996
72	6	0	-3.827192	1.767829	-0.408506
73	6	0	-4.187214	0.359426	-2.365348
74	6	0	-5.192769	1.682937	-0.102270
75	1	0	-3.177309	2.337746	0.250605
76	6	0	-5.556394	0.280013	-2.061692
77	1	0	-3.801730	-0.151459	-3.245647
78	6	0	-6.065628	0.943740	-0.929173
79	1	0	-5.579643	2.191964	0.776500
80	1	0	-6.220979	-0.289426	-2.705899
81	1	0	-7.125199	0.889623	-0.693222
82	6	0	1.315199	3.386912	-1.614179
83	1	0	1.022253	4.286201	-2.179349
84	1	0	2.312812	3.120715	-1.982282
85	6	0	1.415659	3.720353	-0.090509
86	1	0	0.714647	3.096691	0.479248
87	1	0	2.410905	3.424214	0.256343
88	6	0	1.227701	5.202069	0.313996
89	1	0	1.732705	5.870356	-0.394489
90	1	0	1.688032	5.365125	1.296672
91	6	0	-0.261057	5.695942	0.448753
92	1	0	-0.245408	6.696747	0.904148
93	6	0	-1.023512	4.795665	1.346348
94	6	0	-0.948041	5.819105	-0.857757
95	7	0	-1.473564	5.930523	-1.907332
96	7	0	-1.571696	4.024309	2.048770

Acetylenic intermediate of hydroamination, isomer I

E(RB+HF-LYP) = -3416.54760696 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.921019	-1.989414	-3.341883
2	6	0	-3.610286	-1.043583	-2.312593
3	6	0	-2.251092	0.364127	-3.508682
4	6	0	-2.056047	-1.009791	-4.223268
5	1	0	-2.317685	-2.764585	-2.861261
6	1	0	-3.678837	-2.497153	-3.949087
7	1	0	-1.003002	-1.310579	-4.281153
8	1	0	-2.440260	-0.959923	-5.248712
9	6	0	-3.762195	0.271085	-3.146368
10	1	0	-4.142592	1.117022	-2.565093
11	1	0	-4.391679	0.141769	-4.033647
12	6	0	-2.615346	-0.496255	-1.247972

13	1	0	-3.177124	0.277838	-0.701905
14	6	0	-1.529786	0.208534	-2.126207
15	1	0	-0.654012	-0.435770	-2.258872
16	1	0	-4.535412	-1.436064	-1.883689
17	1	0	-1.939292	1.225439	-4.103986
18	15	0	-0.820143	1.640864	-1.101756
19	15	0	-1.819052	-1.374981	0.246985
20	6	0	0.860623	0.748135	2.990692
21	6	0	0.415063	-0.419730	2.850326
22	6	0	-3.283812	-1.669466	1.372014
23	6	0	-4.384276	-2.460912	0.968982
24	6	0	-3.317000	-1.029023	2.629070
25	6	0	-5.494900	-2.614893	1.817758
26	1	0	-4.380618	-2.960903	0.004086
27	6	0	-4.429716	-1.183980	3.477616
28	1	0	-2.484915	-0.403628	2.941982
29	6	0	-5.519475	-1.978220	3.075132
30	1	0	-6.335605	-3.225902	1.499937
31	1	0	-4.444847	-0.686488	4.443822
32	1	0	-6.378693	-2.098831	3.729533
33	6	0	-1.174342	-3.070167	-0.246791
34	6	0	-0.129313	-3.154512	-1.197760
35	6	0	-1.645958	-4.254843	0.357355
36	6	0	0.405102	-4.404724	-1.561513
37	1	0	0.290173	-2.259028	-1.645064
38	6	0	-1.098868	-5.504243	0.002252
39	1	0	-2.431991	-4.218453	1.104826
40	6	0	-0.079079	-5.586466	-0.963171
41	1	0	1.184718	-4.456961	-2.318394
42	1	0	-1.475113	-6.407228	0.475939
43	1	0	0.331944	-6.551998	-1.245664
44	6	0	-2.157136	2.927778	-0.915074
45	6	0	-2.814031	3.079526	0.323467
46	6	0	-2.533888	3.734060	-2.012273
47	6	0	-3.848021	4.024256	0.463528
48	1	0	-2.509291	2.478000	1.176854
49	6	0	-3.566404	4.677341	-1.869208
50	1	0	-2.017944	3.644632	-2.964691
51	6	0	-4.227597	4.821878	-0.632348
52	1	0	-4.347310	4.140576	1.421765
53	1	0	-3.850005	5.298474	-2.714609
54	1	0	-5.023164	5.554361	-0.523831
55	6	0	0.521386	2.456742	-2.101833
56	6	0	1.147570	1.789262	-3.173371
57	6	0	0.943723	3.755375	-1.742546
58	6	0	2.178895	2.423819	-3.890319
59	1	0	0.855808	0.782278	-3.452781
60	6	0	1.974477	4.385418	-2.460116
61	1	0	0.473904	4.277570	-0.912112
62	6	0	2.594037	3.721263	-3.537771
63	1	0	2.656923	1.903762	-4.716215
64	1	0	2.292230	5.385969	-2.179466

65	1	0	3.391839	4.208442	-4.092205
66	16	0	3.398047	-1.010594	-0.517284
67	8	0	3.842269	0.064408	0.596364
68	46	0	-0.255846	0.512130	0.928824
69	1	0	0.516135	1.852186	1.055893
70	6	0	4.976925	-1.189645	-1.774694
71	9	0	4.667758	-2.135979	-2.726584
72	9	0	5.222542	0.020808	-2.374936
73	9	0	6.073171	-1.590735	-1.046163
74	6	0	0.349531	-1.850257	3.280012
75	1	0	0.594631	-1.891430	4.351845
76	1	0	-0.666656	-2.244200	3.165791
77	6	0	1.335228	-2.752408	2.485474
78	1	0	1.031166	-2.724116	1.432868
79	1	0	1.200831	-3.788232	2.827060
80	6	0	2.812219	-2.327821	2.629096
81	1	0	2.896095	-1.236298	2.598683
82	1	0	3.202795	-2.646471	3.606293
83	6	0	3.743866	-2.912845	1.543298
84	1	0	4.764389	-2.542308	1.684489
85	1	0	3.785726	-4.009309	1.597067
86	8	0	2.110313	-0.794836	-1.471095
87	7	0	3.337043	-2.641825	0.136725
88	1	0	2.520148	-3.132060	-0.237753
89	6	0	1.513159	1.942361	3.490242
90	6	0	0.913820	2.686377	4.535851
91	6	0	2.772589	2.339782	2.973758
92	6	0	1.571888	3.809308	5.065520
93	1	0	-0.053018	2.381686	4.928411
94	6	0	3.421755	3.462352	3.510493
95	1	0	3.226231	1.770672	2.165823
96	6	0	2.825467	4.200025	4.554746
97	1	0	1.111624	4.375106	5.871017
98	1	0	4.389637	3.761754	3.117653
99	1	0	3.332584	5.069329	4.965150

Acetylenic intermediate of hydroamination, isomer II

E(RB+HF-LYP) = -3416.54486985 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.833003	-1.004503	-2.469405
2	6	0	3.364731	-1.397906	-2.819760
3	6	0	3.387755	0.883792	-3.043868
4	6	0	4.873241	0.550498	-2.711485
5	1	0	5.110426	-1.268503	-1.447020
6	1	0	5.525424	-1.525312	-3.140307
7	1	0	5.247018	1.101627	-1.839986

8	1	0	5.517559	0.803219	-3.561535
9	6	0	3.019910	-0.346125	-3.925797
10	1	0	1.974053	-0.372893	-4.248958
11	1	0	3.663052	-0.427881	-4.808797
12	6	0	2.339486	-0.912557	-1.753188
13	1	0	1.348599	-1.079759	-2.203199
14	6	0	2.597589	0.628682	-1.711866
15	1	0	3.249738	0.873236	-0.862825
16	1	0	3.236302	-2.446658	-3.100050
17	1	0	3.241327	1.869238	-3.491287
18	15	0	0.971533	1.485508	-1.244186
19	15	0	2.030160	-1.551988	0.015227
20	6	0	-0.234574	0.322490	2.892314
21	6	0	-0.400335	-0.874478	2.555569
22	6	0	1.607060	-3.365475	-0.190524
23	6	0	1.923634	-4.296884	0.824276
24	6	0	0.894426	-3.807201	-1.328172
25	6	0	1.548412	-5.647255	0.695052
26	1	0	2.470513	-3.981636	1.709031
27	6	0	0.520976	-5.157787	-1.455539
28	1	0	0.624973	-3.116393	-2.122565
29	6	0	0.847056	-6.083370	-0.445412
30	1	0	1.807387	-6.353563	1.479512
31	1	0	-0.017378	-5.484238	-2.341539
32	1	0	0.562978	-7.127285	-0.547323
33	6	0	3.615028	-1.502794	1.004749
34	6	0	3.760227	-0.483902	1.971745
35	6	0	4.657795	-2.439031	0.820701
36	6	0	4.939016	-0.392681	2.736603
37	1	0	2.953754	0.225456	2.142133
38	6	0	5.830946	-2.350404	1.590256
39	1	0	4.558102	-3.237339	0.090074
40	6	0	5.975932	-1.324971	2.547454
41	1	0	5.039956	0.394061	3.479489
42	1	0	6.627331	-3.075237	1.443650
43	1	0	6.883696	-1.259617	3.141423
44	6	0	-0.183731	1.466009	-2.703165
45	6	0	-1.393551	0.748420	-2.622985
46	6	0	0.137250	2.179509	-3.880977
47	6	0	-2.278566	0.733552	-3.717968
48	1	0	-1.680746	0.233786	-1.711251
49	6	0	-0.743655	2.154137	-4.975135
50	1	0	1.047671	2.770208	-3.940418
51	6	0	-1.951072	1.427836	-4.896609
52	1	0	-3.218864	0.199466	-3.625392
53	1	0	-0.497279	2.706052	-5.878359
54	1	0	-2.634636	1.420212	-5.741679
55	6	0	1.370337	3.282359	-0.938377
56	6	0	2.698736	3.745286	-0.834864
57	6	0	0.299905	4.191119	-0.783962
58	6	0	2.953438	5.107939	-0.585593
59	1	0	3.540380	3.068828	-0.951949

60	6	0	0.557772	5.550481	-0.538090
61	1	0	-0.729186	3.847256	-0.860154
62	6	0	1.885955	6.012707	-0.437581
63	1	0	3.979766	5.457890	-0.512673
64	1	0	-0.271907	6.243221	-0.426681
65	1	0	2.084594	7.064443	-0.249319
66	16	0	-4.941650	-0.217927	0.000753
67	8	0	-4.041309	-0.376700	-1.329703
68	46	0	0.292514	0.221916	0.671680
69	1	0	-0.734393	1.382081	0.761434
70	6	0	-6.866200	-0.244395	-0.636499
71	9	0	-7.690340	-0.313195	0.463700
72	9	0	-7.123893	0.898599	-1.352433
73	9	0	-7.044992	-1.352706	-1.433633
74	6	0	-0.726271	-2.319828	2.678556
75	1	0	-0.055888	-2.927793	2.061990
76	1	0	-0.541523	-2.602152	3.725738
77	6	0	-2.199861	-2.661023	2.317383
78	1	0	-2.862570	-1.987177	2.879394
79	1	0	-2.402703	-3.682504	2.670660
80	6	0	-2.488789	-2.577680	0.805305
81	1	0	-2.168841	-1.603320	0.409925
82	1	0	-1.892961	-3.339307	0.281354
83	6	0	-3.970301	-2.803583	0.437349
84	1	0	-4.077412	-2.895144	-0.647858
85	1	0	-4.354868	-3.730117	0.884493
86	8	0	-4.796584	1.032992	1.004662
87	7	0	-4.903146	-1.741117	0.891257
88	1	0	-5.019768	-1.573073	1.891769
89	6	0	-0.196112	1.531540	3.690118
90	6	0	-0.684256	1.458664	5.022121
91	6	0	0.320853	2.757306	3.209821
92	6	0	-0.651832	2.591750	5.848874
93	1	0	-1.087308	0.521634	5.397332
94	6	0	0.347227	3.887615	4.042241
95	1	0	0.688931	2.822905	2.190755
96	6	0	-0.136436	3.810476	5.362580
97	1	0	-1.030312	2.528026	6.865520
98	1	0	0.741469	4.825891	3.661604
99	1	0	-0.115827	4.687256	6.004205

Acetylenic intermediate of hydroalkoxylation, isomer I

E(RB+HF-LYP) = -2550.99702256 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.752320	-3.866889	-2.480192
2	6	0	-0.801114	-2.395023	-2.993845
3	6	0	1.407340	-2.714942	-2.484792
4	6	0	0.782397	-4.120038	-2.228232
5	1	0	-1.350946	-4.014877	-1.576978
6	1	0	-1.142054	-4.546636	-3.246245
7	1	0	0.984665	-4.499062	-1.219174
8	1	0	1.184472	-4.849336	-2.941181
9	6	0	0.576821	-2.262333	-3.717809

10	1	0	0.794479	-1.245700	-4.061188
11	1	0	0.681576	-2.950418	-4.563932
12	6	0	-0.544617	-1.361253	-1.854023
13	1	0	-0.452722	-0.384629	-2.355300
14	6	0	0.864810	-1.804415	-1.329264
15	1	0	0.749177	-2.420076	-0.427938
16	1	0	-1.667789	-2.160543	-3.614878
17	1	0	2.493247	-2.720056	-2.602610
18	15	0	1.768426	-0.272356	-0.669923
19	15	0	-1.629302	-0.865276	-0.355249
20	6	0	-1.053883	2.627354	1.543736
21	6	0	-1.302753	1.641399	2.265875
22	6	0	-3.253613	-0.237238	-1.033751
23	6	0	-3.895517	-0.824661	-2.146807
24	6	0	-3.871752	0.852384	-0.380302
25	6	0	-5.127968	-0.323036	-2.604498
26	1	0	-3.450036	-1.671483	-2.657407
27	6	0	-5.109627	1.346446	-0.832228
28	1	0	-3.396284	1.314043	0.480146
29	6	0	-5.739200	0.762663	-1.948030
30	1	0	-5.610319	-0.782070	-3.463469
31	1	0	-5.577642	2.180875	-0.316398
32	1	0	-6.693730	1.145272	-2.299474
33	6	0	-2.049036	-2.409727	0.624735
34	6	0	-1.125081	-2.853695	1.598916
35	6	0	-3.252087	-3.124044	0.438024
36	6	0	-1.386428	-4.012756	2.352383
37	1	0	-0.215613	-2.288842	1.791076
38	6	0	-3.516462	-4.277032	1.200546
39	1	0	-3.989044	-2.783621	-0.282989
40	6	0	-2.581920	-4.729450	2.152741
41	1	0	-0.668262	-4.343435	3.098210
42	1	0	-4.447848	-4.817327	1.052675
43	1	0	-2.788707	-5.620899	2.739019
44	6	0	2.311785	0.761030	-2.124867
45	6	0	1.635462	1.961975	-2.422954
46	6	0	3.385600	0.337559	-2.939277
47	6	0	2.019712	2.728151	-3.539140
48	1	0	0.829793	2.309071	-1.780142
49	6	0	3.767959	1.106996	-4.052025
50	1	0	3.934532	-0.569968	-2.701196
51	6	0	3.082925	2.300979	-4.356569
52	1	0	1.498613	3.655659	-3.760527
53	1	0	4.597348	0.780802	-4.673831
54	1	0	3.383051	2.895431	-5.215524
55	6	0	3.335642	-0.861099	0.146858
56	6	0	3.613456	-2.232232	0.322632
57	6	0	4.254887	0.103442	0.613841
58	6	0	4.806923	-2.634796	0.952748
59	1	0	2.922533	-2.994169	-0.025631
60	6	0	5.446967	-0.301124	1.236826
61	1	0	4.046504	1.164077	0.493289

62	6	0	5.726335	-1.672275	1.408237
63	1	0	5.016442	-3.693545	1.080607
64	1	0	6.151644	0.447529	1.588678
65	1	0	6.649314	-1.984608	1.889706
66	46	0	0.095094	0.751898	0.665492
67	1	0	1.308900	1.590202	1.151804
68	6	0	-1.858946	0.784750	3.344793
69	1	0	-2.454839	1.432824	4.005842
70	1	0	-2.550702	0.054473	2.902733
71	6	0	-0.792319	0.027729	4.179103
72	1	0	-0.230105	-0.651050	3.530530
73	1	0	-1.325978	-0.593780	4.912976
74	6	0	0.203225	0.950033	4.907501
75	1	0	0.705906	1.603796	4.182597
76	1	0	-0.327179	1.594553	5.625101
77	6	0	1.275315	0.160337	5.663053
78	1	0	1.965775	0.851633	6.169148
79	1	0	0.813782	-0.496169	6.418298
80	6	0	-0.890541	3.878606	0.840988
81	6	0	-1.616911	4.140925	-0.348751
82	6	0	-0.017093	4.869632	1.356271
83	6	0	-1.476982	5.376440	-1.001265
84	1	0	-2.288814	3.385781	-0.747264
85	6	0	0.117057	6.102532	0.698673
86	1	0	0.544049	4.668203	2.264694
87	6	0	-0.611435	6.359843	-0.480766
88	1	0	-2.044105	5.575339	-1.906644
89	1	0	0.782648	6.860183	1.102852
90	1	0	-0.508117	7.316603	-0.985803
91	8	0	1.996140	-0.647859	4.668983
92	1	0	2.790034	-1.062874	5.064264

Acetylenic intermediate of hydroalkoxylation, isomer II

E(RB+HF-LYP) = -2550.99698233 A. U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.857903	-1.605878	4.186996
2	6	0	-1.108283	-2.362393	2.845850
3	6	0	1.174970	-2.214359	2.972122
4	6	0	0.710334	-1.593825	4.323437
5	1	0	-1.279232	-0.598367	4.185562
6	1	0	-1.321419	-2.153148	5.015383
7	1	0	1.109118	-0.585608	4.489504
8	1	0	1.040265	-2.220074	5.160479

9	6	0	0.111658	-3.340468	2.806268
10	1	0	0.194384	-3.904689	1.871131
11	1	0	0.122953	-4.045382	3.644740
12	6	0	-0.727575	-1.510499	1.598665
13	1	0	-0.769868	-2.203174	0.743020
14	6	0	0.773488	-1.166526	1.873641
15	1	0	0.847141	-0.159548	2.306508
16	1	0	-2.096129	-2.824383	2.773652
17	1	0	2.221317	-2.526596	2.959614
18	15	0	1.663266	-0.955650	0.209589
19	15	0	-1.595365	0.016256	0.858892
20	6	0	-0.306040	2.477017	-1.945154
21	6	0	-1.254495	1.743349	-2.301228
22	6	0	-3.347897	-0.521615	0.489538
23	6	0	-4.357555	0.456458	0.338844
24	6	0	-3.671192	-1.880075	0.281336
25	6	0	-5.669066	0.079562	-0.002902
26	1	0	-4.130891	1.507976	0.498485
27	6	0	-4.984156	-2.255188	-0.060188
28	1	0	-2.917575	-2.655849	0.383340
29	6	0	-5.987549	-1.278102	-0.203325
30	1	0	-6.437249	0.841335	-0.107382
31	1	0	-5.221305	-3.305683	-0.207683
32	1	0	-7.001869	-1.569388	-0.462544
33	6	0	-1.751347	1.353754	2.156706
34	6	0	-0.837715	2.429805	2.120075
35	6	0	-2.748191	1.321701	3.158035
36	6	0	-0.908262	3.454188	3.083717
37	1	0	-0.087395	2.484449	1.335242
38	6	0	-2.820990	2.349237	4.114804
39	1	0	-3.469131	0.509065	3.190838
40	6	0	-1.898394	3.415275	4.082961
41	1	0	-0.203040	4.280082	3.044274
42	1	0	-3.591419	2.318496	4.880743
43	1	0	-1.958020	4.208708	4.823294
44	6	0	2.025358	-2.628337	-0.527355
45	6	0	1.416232	-3.008495	-1.740930
46	6	0	2.922047	-3.509607	0.119274
47	6	0	1.690300	-4.274268	-2.293772
48	1	0	0.763597	-2.332090	-2.285533
49	6	0	3.188753	-4.772246	-0.436291
50	1	0	3.430417	-3.210601	1.032159
51	6	0	2.568253	-5.159607	-1.642217
52	1	0	1.223362	-4.551776	-3.234264
53	1	0	3.881524	-5.445319	0.061744
54	1	0	2.780302	-6.134967	-2.072620
55	6	0	3.332534	-0.210566	0.589666
56	6	0	3.697856	0.187393	1.892507
57	6	0	4.244954	-0.035103	-0.474532
58	6	0	4.967771	0.749452	2.128885
59	1	0	3.017674	0.062872	2.729647
60	6	0	5.512559	0.521870	-0.234795

61	1	0	3.974559	-0.334858	-1.484604
62	6	0	5.877319	0.916795	1.068595
63	1	0	5.243126	1.049327	3.136576
64	1	0	6.209740	0.647338	-1.058767
65	1	0	6.857903	1.347155	1.253752
66	46	0	0.139614	0.444664	-0.982879
67	1	0	1.317457	0.511979	-1.994037
68	6	0	-2.487557	1.244160	-2.959478
69	1	0	-3.231786	0.956112	-2.204938
70	1	0	-2.906332	2.104489	-3.502841
71	6	0	-2.275973	0.067128	-3.953216
72	1	0	-1.358095	0.226752	-4.530785
73	1	0	-3.115268	0.077317	-4.663713
74	6	0	-2.225259	-1.311593	-3.265472
75	1	0	-1.492008	-1.296432	-2.444690
76	1	0	-3.202996	-1.539327	-2.816576
77	6	0	-1.838524	-2.440927	-4.222614
78	1	0	-2.038159	-3.421611	-3.766054
79	1	0	-2.413240	-2.366792	-5.159201
80	6	0	0.578384	3.610866	-1.773884
81	6	0	0.158670	4.865708	-2.290235
82	6	0	1.829317	3.516425	-1.119312
83	6	0	0.979281	5.995547	-2.152183
84	1	0	-0.799926	4.946115	-2.795816
85	6	0	2.645919	4.651195	-0.987851
86	1	0	2.160424	2.557502	-0.732593
87	6	0	2.225565	5.893572	-1.500715
88	1	0	0.651550	6.951088	-2.552809
89	1	0	3.608151	4.565854	-0.490074
90	1	0	2.859464	6.770219	-1.398043
91	8	0	-0.397352	-2.306960	-4.490177
92	1	0	-0.139635	-2.771218	-5.313108

Acetylenic intermediate of hydrocarbonation, isomer I

$E(\text{RB+HF-LYP}) = -2699.51423298 \quad \text{A. U.}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.965157	-1.134899	-4.445548
2	6	0	-0.484837	-1.119742	-3.875144
3	6	0	0.116625	1.092369	-3.873887
4	6	0	1.344456	0.392205	-4.534713
5	1	0	1.658663	-1.701100	-3.817333
6	1	0	0.971486	-1.599002	-5.438152
7	1	0	2.287975	0.622873	-4.025580
8	1	0	1.446964	0.713106	-5.577868
9	6	0	-1.037906	0.224310	-4.453050
10	1	0	-2.034035	0.482563	-4.079920
11	1	0	-1.056371	0.240701	-5.548361
12	6	0	-0.525805	-0.731148	-2.366814

13	1	0	-1.592376	-0.590191	-2.131593
14	6	0	0.173482	0.670304	-2.365919
15	1	0	1.225349	0.578468	-2.072069
16	1	0	-1.076022	-2.006448	-4.113898
17	1	0	0.065283	2.168481	-4.054014
18	15	0	-0.553143	1.681155	-0.931899
19	15	0	-0.015578	-1.744673	-0.830063
20	6	0	-1.003676	-0.588931	2.963134
21	6	0	0.064322	-1.193610	2.716541
22	6	0	-1.265955	-3.133192	-0.786485
23	6	0	-1.482552	-3.978041	-1.899942
24	6	0	-2.040173	-3.316158	0.379293
25	6	0	-2.458124	-4.989245	-1.844171
26	1	0	-0.894418	-3.859996	-2.805494
27	6	0	-3.014583	-4.331035	0.434266
28	1	0	-1.888860	-2.668753	1.237764
29	6	0	-3.226248	-5.168817	-0.676279
30	1	0	-2.617103	-5.632750	-2.705367
31	1	0	-3.606557	-4.462746	1.336172
32	1	0	-3.979710	-5.950909	-0.635171
33	6	0	1.658962	-2.547650	-1.109580
34	6	0	2.805733	-1.722554	-1.184862
35	6	0	1.813597	-3.947677	-1.203453
36	6	0	4.077123	-2.287271	-1.391775
37	1	0	2.724451	-0.645113	-1.075186
38	6	0	3.090713	-4.511072	-1.392957
39	1	0	0.953036	-4.604586	-1.126552
40	6	0	4.224771	-3.684536	-1.498331
41	1	0	4.946844	-1.639345	-1.471392
42	1	0	3.194802	-5.590684	-1.462822
43	1	0	5.207265	-4.121078	-1.657043
44	6	0	-2.349990	2.015953	-1.308952
45	6	0	-3.355413	1.352455	-0.575617
46	6	0	-2.710499	2.915158	-2.337746
47	6	0	-4.712487	1.577871	-0.873294
48	1	0	-3.084467	0.678124	0.233172
49	6	0	-4.066828	3.138145	-2.632501
50	1	0	-1.947339	3.451996	-2.895103
51	6	0	-5.070256	2.467525	-1.903415
52	1	0	-5.481829	1.066610	-0.300952
53	1	0	-4.339176	3.832984	-3.422377
54	1	0	-6.117955	2.644215	-2.132096
55	6	0	0.268228	3.351069	-0.926676
56	6	0	1.510303	3.558984	-1.558462
57	6	0	-0.359471	4.418262	-0.247187
58	6	0	2.109277	4.831797	-1.529418
59	1	0	2.019472	2.751594	-2.073543
60	6	0	0.245363	5.686008	-0.213818
61	1	0	-1.317336	4.270220	0.246212
62	6	0	1.481411	5.896682	-0.857444
63	1	0	3.066084	4.985873	-2.021070
64	1	0	-0.245174	6.503772	0.307310

65	1	0	1.948239	6.877788	-0.833544
66	46	0	-0.285131	0.148549	0.887802
67	1	0	-0.437934	1.469528	1.691529
68	6	0	1.228380	-2.091963	2.940540
69	1	0	1.127690	-2.486271	3.963335
70	1	0	1.168288	-2.952380	2.260206
71	6	0	2.622655	-1.429984	2.784780
72	1	0	2.805356	-1.264353	1.716386
73	1	0	3.369236	-2.159798	3.131697
74	6	0	2.766225	-0.104741	3.564106
75	1	0	2.079664	0.638044	3.137275
76	1	0	2.452559	-0.253909	4.607348
77	6	0	4.197956	0.476163	3.592237
78	1	0	4.177280	1.477700	4.036575
79	1	0	4.854896	-0.142885	4.216298
80	6	0	-2.249312	-0.158088	3.564896
81	6	0	-3.089794	-1.150873	4.135502
82	6	0	-2.632535	1.202263	3.648353
83	6	0	-4.278152	-0.782672	4.786889
84	1	0	-2.800120	-2.197127	4.079673
85	6	0	-3.820446	1.562454	4.303058
86	1	0	-2.000147	1.965253	3.204429
87	6	0	-4.647560	0.574209	4.873898
88	1	0	-4.910674	-1.548512	5.227607
89	1	0	-4.101559	2.609974	4.368655
90	1	0	-5.566866	0.857412	5.379275
91	6	0	4.884147	0.566315	2.179558
92	1	0	5.140542	-0.453865	1.857509
93	6	0	6.142215	1.339325	2.242296
94	6	0	3.978044	1.113474	1.144715
95	7	0	7.152442	1.942241	2.317898
96	7	0	3.209301	1.464566	0.326232

Acetylenic intermediate of hydrocarbonation, isomer II

$E(\text{RB+HF-LYP}) = -2699.51459021 \quad \text{A. U.}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.659904	4.076094	1.104204
2	6	0	1.427150	3.457141	1.831813
3	6	0	3.105780	1.942947	2.215956
4	6	0	3.834256	3.084763	1.445573
5	1	0	2.508474	4.179447	0.027971
6	1	0	2.860822	5.076640	1.503245
7	1	0	4.356116	2.727428	0.549539
8	1	0	4.580278	3.561026	2.092205
9	6	0	2.106669	2.780255	3.068534
10	1	0	1.419781	2.182156	3.676547

11	1	0	2.619675	3.496537	3.719482
12	6	0	0.913397	2.155464	1.148068
13	1	0	0.187643	1.724229	1.854488
14	6	0	2.185396	1.247057	1.151351
15	1	0	2.681022	1.297406	0.172833
16	1	0	0.632438	4.173566	2.055673
17	1	0	3.776969	1.275171	2.760065
18	15	0	1.619336	-0.561539	1.236793
19	15	0	-0.027786	1.936250	-0.494096
20	6	0	-0.677934	-1.735141	-2.364891
21	6	0	-1.550896	-0.848581	-2.185298
22	6	0	-1.570772	2.980926	-0.306188
23	6	0	-2.172292	3.582416	-1.434717
24	6	0	-2.190379	3.118773	0.956137
25	6	0	-3.363625	4.319591	-1.299752
26	1	0	-1.711966	3.495498	-2.415523
27	6	0	-3.380623	3.857116	1.089201
28	1	0	-1.760893	2.661487	1.843336
29	6	0	-3.971963	4.460834	-0.037612
30	1	0	-3.809159	4.784661	-2.175262
31	1	0	-3.839089	3.963683	2.068865
32	1	0	-4.888187	5.035585	0.067118
33	6	0	0.937430	2.696211	-1.902601
34	6	0	1.587472	1.824859	-2.803761
35	6	0	1.033728	4.093300	-2.095253
36	6	0	2.337427	2.342443	-3.877260
37	1	0	1.496782	0.748291	-2.680419
38	6	0	1.777677	4.607850	-3.171483
39	1	0	0.529025	4.778812	-1.419557
40	6	0	2.434524	3.733968	-4.062452
41	1	0	2.832474	1.663432	-4.566374
42	1	0	1.845916	5.683088	-3.313697
43	1	0	3.008196	4.135079	-4.893759
44	6	0	1.030274	-0.963069	2.955182
45	6	0	-0.316659	-1.323119	3.159822
46	6	0	1.926626	-0.936213	4.048235
47	6	0	-0.774134	-1.649260	4.450592
48	1	0	-1.009617	-1.384796	2.326194
49	6	0	1.465050	-1.251831	5.337320
50	1	0	2.976540	-0.698339	3.898926
51	6	0	0.114173	-1.605684	5.540383
52	1	0	-1.809470	-1.946694	4.577206
53	1	0	2.155706	-1.233335	6.176226
54	1	0	-0.234926	-1.859394	6.537979
55	6	0	3.136077	-1.615061	0.965188
56	6	0	4.335063	-1.074213	0.455479
57	6	0	3.063447	-2.994163	1.261904
58	6	0	5.453607	-1.905068	0.251083
59	1	0	4.419447	-0.016996	0.221882
60	6	0	4.182291	-3.820186	1.058755
61	1	0	2.146462	-3.423549	1.658936
62	6	0	5.380851	-3.277773	0.552167

63	1	0	6.375521	-1.479122	-0.135826
64	1	0	4.119766	-4.878333	1.297836
65	1	0	6.246589	-3.916431	0.398636
66	46	0	-0.048399	-0.627642	-0.483591
67	1	0	0.073401	-2.139886	-0.152412
68	6	0	-2.755922	-0.035451	-2.505302
69	1	0	-2.588717	1.021530	-2.271292
70	1	0	-2.897258	-0.102771	-3.594329
71	6	0	-4.060073	-0.511564	-1.801008
72	1	0	-4.121850	-1.606910	-1.868438
73	1	0	-4.910315	-0.110213	-2.370793
74	6	0	-4.175667	-0.032195	-0.338297
75	1	0	-3.290945	-0.347001	0.233924
76	1	0	-4.168855	1.065660	-0.330483
77	6	0	-5.463721	-0.506220	0.372256
78	1	0	-5.668774	0.119433	1.248562
79	1	0	-6.326601	-0.414858	-0.299705
80	6	0	0.031970	-2.854045	-2.954328
81	6	0	-0.615714	-3.575624	-3.992464
82	6	0	1.339205	-3.228177	-2.564389
83	6	0	0.037995	-4.645942	-4.622159
84	1	0	-1.621585	-3.297231	-4.295861
85	6	0	1.985755	-4.301815	-3.197150
86	1	0	1.839275	-2.682451	-1.770196
87	6	0	1.340293	-5.013452	-4.227126
88	1	0	-0.465221	-5.194032	-5.414138
89	1	0	2.989053	-4.582325	-2.888451
90	1	0	1.842759	-5.844229	-4.715141
91	6	0	-5.394520	-2.000772	0.852512
92	1	0	-5.152428	-2.644419	-0.005577
93	6	0	-4.317932	-2.161813	1.855262
94	6	0	-6.692562	-2.451260	1.399327
95	7	0	-3.427407	-2.215985	2.622332
96	7	0	-7.743985	-2.792808	1.808726

Full reference 41:

41. Gaussian 03, Revision B.05, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V.

G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.