Supporting Information

Stereoselective Hydrocoupling of Cinnamic Acid Esters by Electroreduction: Application to Asymmetric Synthesis of Hydrodimers

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Compounds Characterization Data

1k: *R_f* 0.6 (hexane-ethyl acetate, 10:1). mp 65-67 °C. $[\alpha]_D^{25}$ 9.4 (*c* 1.1, CHCl₃). IR (KBr) 1705, 1641, 1495, 986, 764, 696, 681 cm⁻¹. ¹H NMR (CDCl₃) δ 0.89 (d, 3 H, *J* = 6.8 Hz), 0.90-1.28 (m, 3 H), 1.23 (s, 3 H), 1.33 (s, 3 H), 1.44-1.61 (m, 1 H), 1.62-1.83 (m, 2 H), 1.90-2.00 (m, 1 H), 2.06-2.17 (m, 1 H), 4.91 (dt, 1 H, *J* = 4.3, 10.8 Hz), 5.75 (d, 1 H, *J* = 16.2 Hz), 7.04-7.12 (m, 1 H), 7.17-7.42 (m, 10 H). ¹³C NMR (CDCl₃) δ 21.74 (q), 24.30 (q), 26.49 (t), 28.36 (q), 31.24 (d), 34.61 (t), 39.56 (s), 41.72 (t), 50.68 (d), 74.24 (d), 118.78 (d), 124.72 (d), 125.38 (d), 127.88 (d), 128.63 (d), 129.81 (d), 134.56 (s), 143.49 (d), 151.73 (s), 165.92 (s). Anal. Calcd for C₂₅H₃₀O₂: C, 82.83; H, 8.34. Found: C, 82.74; H, 8.40.

1m: *R_f* 0.65 (hexane-ethyl acetate, 10:1). $[\alpha]_D^{20}$ -76.2 (*c* 2.85, CHCl₃). IR (KBr) 1709, 1638, 1578, 1497, 768, 710, 685 cm⁻¹. ¹H NMR (CDCl₃) δ 0.87 (s, 3 H), 0.90 (s, 3 H), 1.06 (s, 3 H), 1.07-1.28 (m, 2 H), 1.52-1.92 (m, 5 H), 4.81 (dd, 1 H, *J* = 4.3, 7.0 Hz), 6.41 (d, 1 H, *J* = 15.9 Hz), 7.34-7.41 (m, 3 H), 7.48-7.56 (m, 2 H), 7.63 (d, 1 H, *J* = 15.9 Hz). ¹³C NMR (CDCl₃) δ 11.55 (q), 20.04 (q), 20.18 (q), 27.10 (t), 33.76 (t), 38.86 (t), 45.08 (d), 46.96 (s), 48.86 (s), 80.97 (d), 118.75 (d), 127.86 (d), 128.65 (d), 129.95 (d), 134.36 (s), 143.99 (d), 166.21 (s). Anal. Calcd for C₁₉H₂₄O₂: C, 80.24; H, 8.51. Found: C, 80.21; H, 8.56.

1n: *R_f* 0.57 (hexane-ethyl acetate, 10:1). $[\alpha]_D^{20}$ 20.1 (*c* 1.05, CHCl₃). IR (KBr) 1715, 1639, 1578, 1497, 980, 768, 700, 684 cm⁻¹. ¹H NMR (CDCl₃) δ 0.84 (s, 3 H), 0.90 (s, 3 H), 0.94-1.05 (m, 1 H), 1.22-1.35 (m, 1 H), 1.31 (s, 3 H), 1.49-1.75 (m, 3 H), 2.22-2.33 (m, 1 H), 2.66-2.87 (m, 2 H), 5.16 (d, 1 H, *J* = 8.1 Hz), 6.44 (d, 1 H, *J* = 16.2 Hz), 7.10-7.19 (m, 3 H), 7.21-7.28 (m, 2 H), 7.35-7.42 (m, 3 H), 7.50-7.57 (m, 2 H), 7.66 (d, 1 H, *J* = 16.2 Hz). ¹³C NMR (CDCl₃) δ 11.75 (q), 21.62 (q), 21.93 (q), 29.70 (t), 33.31 (t), 36.17 (t), 47.43 (s), 48.26 (d), 49.92 (s), 51.04 (s), 82.40 (d), 118.30 (d), 125.50 (d), 127.92 (d), 128.10 (d), 128.69 (d), 128.72 (d), 130.06 (d), 134.27 (s), 141.75 (s), 144.36 (d), 166.43 (s). Anal. Calcd for C₂₆H₃₀O₂: C, 83.38; H, 8.07. Found: C, 83.25; H, 8.18.

meso-3a:¹ *R_f* 0.40 (hexane-ethyl acetate, 5:1). mp 174-176 °C (lit.¹ 175-177 °C). IR (KBr) 1725, 705 cm⁻¹. ¹H NMR (CDCl₃) δ 2.30-2.54 (m, 4 H), 3.22-3.40 (m, 2 H), 3.36 (s, 6 H), 7.02-7.46 (m, 10 H). ¹³C NMR (CDCl₃) δ 39.60 (t), 47.59 (d), 51.20 (q), 127.23 (d), 128.25 (d), 128.80 (d), 141.86 (s), 172.65 (s).

meso-3b: *Rf* 0.24 (hexane-ethyl acetate, 5:1). mp 143-144 °C. IR (KBr) 1744, 1599, 1587, 1495, 754, 739 cm⁻¹. ¹H NMR (CDCl₃) δ 2.30-2.39 (m, 2 H), 2.60-2.73 (m, 2 H), 3.32 (s, 3 H), 3.85-3.90 (m, 2 H), 3.88 (s, 3 H), 6.84-6.96 (m, 4 H), 7.16-7.28 (m, 4 H). ¹³C NMR (CDCl₃) δ 37.95 (t), 51.05 (q), 55.59 (q), 110.88 (d), 120.58 (d), 127.64 (d), 130.30 (s), 157.75 (s), 172.76 (s). Anal. Calcd for C₂₂H₂₆O₆: C, 68.38; H, 6.78. Found: C, 68.45; H, 6.82.

meso-3c: *Rf* 0.22 (hexane-ethyl acetate, 5:1). mp 138 °C. IR (KBr) 1722, 1597, 1489, 797. 704 cm⁻¹. ¹H NMR (CDCl₃) δ 2.34-2.52 (m, 4 H), 3.20-3.33 (m, 2 H), 3.39 (s, 6 H), 3.81 (s, 6 H), 6.75-6.82 (m, 4 H), 6.84-6.90 (m, 2 H), 7.24 (t, 2 H, *J* = 7.8 Hz). ¹³C NMR (CDCl₃) δ 39.68 (t), 47.73 (d), 51.35 (q), 55.22 (q), 112.26 (d), 113.96 (d), 120.39 (d), 129.53 (d), 143.26 (s), 159.61 (s), 172.15 (s). Anal. Calcd for C₂₂H₂₆O₆: C, 68.38; H, 6.78. Found: C, 68.38; H, 6.84.

meso-3d: *Rf* 0.19 (hexane-ethyl acetate, 2:1). mp 157-158 °C. IR (KBr) 1720, 1614, 1518, 837, 827, 714 cm⁻¹. ¹H NMR (CDCl₃) δ 2.33-2.43 (m, 4 H), 3.15-3.28 (m, 2 H), 3.38 (s, 6 H), 3.79 (s, 6 H), 6.82-6.89 (m, 4 H), 7.14-7.21 (m, 4 H). ¹³C NMR (CDCl₃) δ 39.90 (t), 47.18 (d), 51.31 (q), 55.22 (q), 113.97 (d), 128.93 (d), 133.67 (s), 158.38 (s), 172.38 (s). Anal. Calcd for C₂₂H₂₆O₆: C, 68.38; H, 6.78. Found: C, 68.42; H, 6.76.

meso-3e: *Rf* 0.26 (hexane-ethyl acetate, 5:1). mp 148 °C. IR (KBr) 1732, 1605, 1508, 835, 723, 714 cm⁻¹. ¹H NMR (CDCl₃) δ 2.30-2.47 (m, 4 H), 3.23-3.35 (m, 2 H), 3.40 (s, 6 H), 6.97-7.07 (m, 4 H), 7.18-7.26 (m, 4 H). ¹³C NMR (CDCl₃) δ 39.66 (t), 47.05 (d), 51.45 (q), 115.52 (d, *J*_{CCF} = 21.1 Hz), 129.48 (d, *J*_{CCCF} = 7.8 Hz), 137.05 (s, *J*_{CCCCF} = 3.3 Hz), 161.73 (s, *J*_{CF} = 243.8 Hz), 171.92 (s). Anal. Calcd for C₂₀H₂₀F₂O₄: C, 66.29; H, 5.56. Found: C, 66.25; H, 5.60.

meso-3f: *Rf* 0.28 (hexane-ethyl acetate, 5:1). mp 219-220 °C. IR (KBr) 1753, 1728, 1601, 1508, 856, 824, 743 cm⁻¹. ¹H NMR (CDCl₃) δ 2.45 (dd, 2 H, *J* = 3.8, 15.7 Hz), 2.56-2.67 (m, 2 H), 3.26 (s, 6 H), 3.55-3.68 (m, 2 H), 7.42-7.53 (m, 6 H), 7.78-7.88 (m, 8 H). ¹³C NMR (CDCl₃) δ 39.81 (t), 47.83 (d), 51.30 (q), 125.68 (d), 125.72 (d), 126.05 (d), 127.33 (d), 127.55 (d), 127.72 (d), 128.49 (d), 132.63 (s), 133.39 (s), 139.09 (s), 172.08 (s). Anal. Calcd for C₂₈H₂₆O₄: C, 78.85; H, 6.14. Found: C, 78.91; H, 6.16.

meso-3h: *Rf* 0.23 (hexane-ethyl acetate, 5:1). mp 203-204 °C. IR (KBr) 1732, 1605, 1501, 1487, 931, 903, 874, 822, 750 cm⁻¹. ¹H NMR (CDCl₃) δ 2.33-2.43 (m, 4 H), 3.08-3.21 (m, 2 H), 3.43 (s, 6 H), 5.94 (s, 4 H), 6.68-6.77 (m, 6 H). ¹³C NMR (CDCl₃) δ

39.85 (t), 47.70 (d), 51.40 (q), 100.94 (t), 107.90 (d), 108.28 (d), 121.44 (d), 135.34 (s), 146.43 (s), 147.79 (s), 172.18 (s). Anal. Calcd for $C_{22}H_{22}O_8$: C, 63.76; H, 5.35. Found: C, 63.73; H, 5.39.

meso-**3i**: *Rf* 0.17 (hexane-ethyl acetate, 5:1). mp 217-218 °C. IR (KBr) 1732, 1618, 1523, 816 cm^{-1} . 1H NMR ($CDCl_3$) δ 2.33-2.43 (m, 4 H), 2.92 (s, 12 H), 3.09-3.21 (m, 2 H), 3.38 (s, 6 H), 6.65-6.72 (m, 4 H), 7.09-7.16 (m, 4 H). ^{13}C NMR ($CDCl_3$) δ 40.08 (t), 40.69 (q), 47.18 (d), 51.22 (q), 112.74 (d), 128.58 (d), 129.81 (s), 149.37 (s), 172.77 (s). Anal. Calcd for $C_{24}H_{32}N_2O_4$: C, 69.88; H, 7.82; N, 6.79. Found: C, 69.64; H, 7.94; N, 6.62.

dl-**3a**:¹ *Rf* 0.30 (hexane-ethyl acetate, 5:1). mp 71-73 °C (lit.¹ 72-74 °C). IR (neat) 1725, 700 cm^{-1} . 1H NMR ($CDCl_3$) δ 2.54-2.81 (m, 4 H), 3.42-3.58 (m, 2 H), 3.55 (s, 6 H), 6.82-6.96 (m, 4 H), 7.10-7.24 (m, 6 H). ^{13}C NMR ($CDCl_3$) δ 37.47 (t), 46.14 (d), 51.52 (q), 126.86 (d), 127.98 (d), 128.90 (d), 140.19 (s), 172.76 (s).

dl-**3b**:² *Rf* 0.57 (hexane-ethyl acetate, 2:1). IR (neat) 1739, 1732, 754 cm^{-1} . 1H NMR ($CDCl_3$) δ 2.61-2.77 (m, 4 H), 3.51 (s, 6 H), 3.75 (s, 6 H), 4.01-4.13 (m, 2 H), 6.65-6.75 (m, 6 H), 7.03-7.10 (m, 2 H). ^{13}C NMR ($CDCl_3$) δ 37.05 (t), 39.01 (d), 51.25 (q), 55.11 (q), 110.15 (d), 119.60 (d), 127.28 (d), 129.39 (s), 129.59 (d), 157.35 (s), 173.02 (s).

dl-**3c**:² *Rf* 0.58 (hexane-ethyl acetate, 2:1). IR (neat) 1750, 1732, 785, 702 cm^{-1} . 1H NMR ($CDCl_3$) δ 2.55-2.78 (m, 4 H), 3.42-3.53 (m, 2 H), 3.57 (s, 6 H), 3.68 (s, 6 H), 6.41 (t, 2 H, J = 1.9 Hz), 6.53 (d, 2 H, J = 7.8 Hz), 6.67-6.74 (m, 2 H), 7.10 (t, 2 H, J = 7.8 Hz). ^{13}C NMR ($CDCl_3$) δ 37.34 (t), 46.01 (d), 51.44 (q), 54.87 (q), 112.30 (d), 114.31 (d), 121.07 (d), 128.66 (d), 141.58 (s), 158.96 (s), 172.28 (s).

dl-**3d**:² *Rf* 0.53 (hexane-ethyl acetate, 2:1). IR (neat) 1750, 1732, 1717, 814 cm^{-1} . 1H NMR ($CDCl_3$) δ 2.48-2.60 (m, 2 H), 2.63-2.75 (m, 2 H), 3.35-3.47 (m, 2 H), 3.55 (s, 6 H), 3.75 (s, 6 H), 6.69-6.80 (m, 8 H). ^{13}C NMR ($CDCl_3$) δ 37.93 (t), 45.42 (d), 51.39 (q), 54.97 (q), 113.13 (d), 129.73 (d), 131.89 (s), 158.23 (s), 172.48 (s).

dl-**3e**:² *Rf* 0.62 (hexane-ethyl acetate, 2:1). IR (neat) 1750, 1732, 837 cm^{-1} . 1H NMR ($CDCl_3$) δ 2.52-2.63 (m, 2 H), 2.68-2.79 (m, 2 H), 3.38-3.49 (m, 2 H), 3.56 (s, 6 H), 6.76-7.12 (m, 8 H). ^{13}C NMR ($CDCl_3$) δ 38.12 (t), 45.62 (d), 51.59 (q), 114.70 (d, J_{CCF} = 19.8 Hz), 130.03 (d, J_{CCCF} = 6.6 Hz), 135.56 (s), 161.56 (s, J_{CF} = 244.6 Hz), 172.09 (s).

dl-3f: *Rf* 0.37 (hexane-ethyl acetate, 2:1). mp 148-149 °C. IR (KBr) 1736, 1599, 1508, 862, 827, 756 cm⁻¹. ¹H NMR (CDCl₃) δ 2.69-2.91 (m, 4 H), 3.51 (s, 6 H), 3.77-3.82 (m, 2 H), 7.05 (dd, 2 H, *J* = 1.6, 8.1 Hz), 7.36-7.45 (m, 6 H), 7.62-7.69 (m, 4 H), 7.73-7.78 (m, 2 H). ¹³C NMR (CDCl₃) δ 37.58 (t), 46.35 (d), 51.69 (q), 125.49 (d), 125.77 (d), 127.01 (d), 127.38 (d), 127.65 (d), 132.31 (s), 132.88 (s), 137.46 (s), 172.24 (s). Anal. Calcd for C₂₈H₂₆O₄: C, 78.85; H, 6.14. Found: C, 78.82; H, 6.16.

dl-3g: *Rf* 0.31 (hexane-ethyl acetate, 5:1). IR (neat) 1738, 1591, 1504, 810, 734 cm⁻¹. ¹H NMR (CDCl₃) δ 2.60-2.70 (m, 4 H), 3.61 (s, 6 H), 3.63-3.80 (m, 2 H), 5.96 (d, 2 H, *J* = 3.2 Hz), 6.22-6.27 (m, 2 H), 7.23-7.35 (m, 2 H). ¹³C NMR (CDCl₃) δ 34.89 (t), 38.60 (d), 51.60 (q), 106.44 (d), 109.85 (d), 141.28 (d), 153.91 (s), 171.71 (s). Anal. Calcd for C₁₆H₁₈O₆: C, 62.74; H, 5.92. Found: C, 62.85; H, 6.08.

dl-3h: *Rf* 0.52 (hexane-ethyl acetate, 2:1). mp 104-105 °C. IR (KBr) 1732, 1611, 1502, 1489, 814, 733 cm⁻¹. ¹H NMR (CDCl₃) δ 2.48-2.62 (m, 2 H), 2.64-2.76 (m, 2 H), 3.29-3.45 (m, 2 H), 3.57 (s, 6 H), 5.88-5.94 (m, 4 H), 6.33-6.42 (m, 2 H), 6.50-6.80 (m, 4 H). ¹³C NMR (CDCl₃) δ 37.99 (t), 46.15 (d), 51.61 (q), 100.73 (t), 107.60 (d), 108.87 (d), 121.72 (d), 133.79 (s), 146.03 (s), 147.02 (s), 172.14 (s). Anal. Calcd for C₂₂H₂₂O₈: C, 63.76; H, 5.35. Found: C, 63.60; H, 5.26.

10a:³ *Rf* 0.45 (hexane-ethyl acetate, 5:1). mp 181-183 °C (lit.³ 180-183 °C). IR (KBr) 1735, 760, 695 cm⁻¹. ¹H NMR (CDCl₃) δ 2.48-2.67 (m, 2 H), 2.79-2.96 (m, 2 H), 3.40-3.56 (m, 2 H), 7.08-7.28 (m, 10 H). ¹³C NMR (CDCl₃) δ 47.17 (t), 50.11 (d), 126.84 (d), 127.19 (d), 128.56 (d), 140.85 (s), 215.74 (s).

10b: *Rf* 0.4 (hexane-ethyl acetate, 5:1). IR (KBr) 1736, 1601, 1495, 750 cm⁻¹. ¹H NMR (CDCl₃) δ 2.35-2.52 (m, 2 H), 2.84-2.96 (m, 2 H), 3.78 (s, 6 H), 3.94-4.08 (m, 2 H), 6.79-6.86 (m, 2 H), 7.10-7.18 (m, 2 H). ¹³C NMR (CDCl₃) δ 41.58 (d), 46.12 (t), 55.22 (q), 110.46 (d), 120.48 (d), 127.35 (d), 127.42 (d), 130.12 (s), 157.39 (s), 217.73 (s). Anal. Calcd for C₁₉H₂₀O₃: C, 77.00; H, 6.80. Found: C, 76.95; H, 6.82.

10c: *Rf* 0.27 (hexane-ethyl acetate, 5:1). IR (neat) 1744, 1601, 1585, 1489, 781, 729, 698 cm⁻¹. ¹H NMR (CDCl₃) δ 2.46-2.64 (m, 2 H), 2.79-2.92 (m, 2 H), 3.39-3.54 (m, 2 H), 3.72 (s, 6 H), 6.66 (t, 2 H, *J* = 1.9 Hz), 6.69-6.76 (m, 4 H), 7.17 (t, 2 H, *J* = 8.1 Hz). ¹³C NMR (CDCl₃) δ 47.21 (t), 49.91 (d), 55.12 (q), 111.86 (d), 113.27 (d), 119.38 (d), 129.44 (d), 142.48 (s), 159.49 (s), 215.36 (s). Anal. Calcd for C₁₉H₂₀O₃: C, 77.00; H, 6.80. Found: C, 76.88; H, 6.87.

10d: *Rf* 0.3 (hexane-ethyl acetate, 5:1). IR (neat) 1738, 1612, 1583, 1514, 829, 789, 775, 731 cm^{-1} . ^1H NMR (CDCl_3) δ 2.43-2.61 (m, 2 H), 2.76-2.88 (m, 2 H), 3.30-3.45 (m, 2 H), 3.75 (s, 6 H), 6.74-6.81 (m, 4 H), 6.99-7.06 (m, 4 H). ^{13}C NMR (CDCl_3) δ 47.30 (t), 49.56 (d), 55.12 (q), 113.76 (d), 128.00 (d), 132.78 (s), 158.13 (s), 215.71 (s). Anal. Calcd for $\text{C}_{19}\text{H}_{20}\text{O}_3$: C, 77.00; H, 6.80. Found: C, 76.85; H, 6.73.

10e: *Rf* 0.38 (hexane-ethyl acetate, 5:1). IR (KBr) 1747, 1605, 1514, 835, 818, 795 cm^{-1} . ^1H NMR (CDCl_3) δ 2.44-2.63 (m, 2 H), 2.79-2.92 (m, 2 H), 3.32-3.47 (m, 2 H), 6.88-6.98 (m, 4 H), 7.01-7.09 (m, 4 H). ^{13}C NMR (CDCl_3) δ 47.10 (t), 49.89 (d), 115.34 (d, $J_{\text{CCF}} = 21.1$ Hz), 128.47 (d, $J_{\text{CCCF}} = 7.8$ Hz), 136.04 (s, $J_{\text{CCCCF}} = 3.3$ Hz), 161.52 (s, $J_{\text{CF}} = 243.8$ Hz), 214.55 (s). Anal. Calcd for $\text{C}_{17}\text{H}_{14}\text{F}_2\text{O}$: C, 74.99; H, 5.18. Found: C, 75.14; H, 5.30.

10f: *Rf* 0.55 (hexane-ethyl acetate, 5:1). mp 225 $^{\circ}\text{C}$. IR (KBr) 1728, 1601, 1508, 824, 743 cm^{-1} . ^1H NMR (CDCl_3) δ 2.67-2.81 (m, 2 H), 2.92-3.05 (m, 2 H), 3.72-3.87 (m, 2 H), 7.29 (dd, 2 H, $J = 1.6, 8.6$ Hz), 7.36-7.44 (m, 4 H), 7.58 (d, 2 H, $J = 1.4$ Hz), 7.64-7.80 (m, 6 H). ^{13}C NMR (CDCl_3) δ 47.25 (t), 50.10 (d), 125.18 (d), 125.52 (d), 125.81 (d), 125.98 (d), 127.42 (d), 127.42 (d), 128.22 (d), 132.32 (s), 133.21 (s), 138.20 (s), 215.23 (s). Anal. Calcd for $\text{C}_{25}\text{H}_{20}\text{O}$: C, 89.25; H, 5.99. Found: C, 89.26; H, 6.03.

10g: *Rf* 0.8 (hexane-ethyl acetate, 2:1). IR (neat) 1732, 1715, 1599, 1506, 928, 912, 883, 810, 739 cm^{-1} . ^1H NMR (CDCl_3) δ 2.50-2.66 (m, 2 H), 2.68-2.85 (m, 2 H), 3.62-3.75 (m, 2 H), 6.04 (d, 2 H, $J = 3.2$ Hz), 6.28 (dd, 2 H, $J = 1.9, 3.2$ Hz), 7.34 (dd, 2 H, $J = 0.8, 1.9$ Hz). ^{13}C NMR (CDCl_3) δ 40.78 (d), 43.37 (t), 105.78 (d), 110.11 (d), 141.54 (d), 154.36 (s), 214.70 (s). Anal. Calcd for $\text{C}_{13}\text{H}_{12}\text{O}_3$: C, 72.21; H, 5.59. Found: C, 72.07; H, 5.72.

10h: *Rf* 0.27 (hexane-ethyl acetate, 5:1). mp 139-140 $^{\circ}\text{C}$. IR (KBr) 1732, 1609, 1504, 1489, 932, 870, 814 cm^{-1} . ^1H NMR (CDCl_3) δ 2.37-2.56 (m, 2 H), 2.75-2.87 (m, 2 H), 3.26-3.41 (m, 2 H), 5.91 (s, 4 H), 6.56 (dd, 2 H, $J = 1.6, 8.1$ Hz), 6.64 (d, 2 H, $J = 1.6$ Hz), 6.68 (d, 2 H, $J = 8.1$ Hz). ^{13}C NMR (CDCl_3) δ 47.46 (t), 49.98 (d), 100.84 (t), 107.10 (d), 108.09 (d), 120.35 (d), 134.45 (s), 146.14 (s), 147.59 (s), 215.14 (s). Anal. Calcd for $\text{C}_{19}\text{H}_{16}\text{O}_5$: C, 70.36; H, 4.97. Found: C, 70.39; H, 4.93.

13a: *Rf* 0.4, 0.5 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.72 (s, 1.5 H), 0.73 (s, 1.5 H), 0.76 (s, 3 H), 1.00-1.12 (m, 1 H), 1.26 (s, 1.5 H), 1.27 (s, 1.5 H), 1.28-1.72 (m, 4 H), 1.90 (dd, 0.5 H, $J = 2.3, 16.7$ Hz), 1.93 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.16 (dd,

0.5 H, $J = 3.2, 16.7$ Hz), 2.29 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.75 (brs, 0.5 H), 2.83 (dd, 1 H, $J = 8.1, 13.0$ Hz), 3.38 (brs, 0.5 H), 4.27 (d, 1 H, $J = 13.0$ Hz), 4.45 (dd, 0.5 H, $J = 2.3, 10.0$ Hz), 4.81 (d, 0.5 H, $J = 3.2, 10.0$ Hz), 5.25 (d, 0.5 H, $J = 8.1$ Hz), 5.28 (d, 0.5 H, $J = 8.1$ Hz), 7.00-7.74 (m, 15 H).

13b: R_f 0.38 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.66 (s, 1.2 H), 0.74 (s, 1.2 H), 0.75 (s, 1.8 H), 0.77 (s, 1.8 H), 1.02-1.13 (m, 1 H), 1.25 (s, 1.2 H), 1.31 (s, 1.8 H), 1.27-1.73 (m, 4 H), 1.94 (dd, 0.6 H, $J = 9.7, 16.2$ Hz), 2.16 (dd, 0.4 H, $J = 3.2, 16.2$ Hz), 2.289 (dd, 0.6 H, $J = 3.2, 16.2$ Hz), 2.294 (dd, 0.4 H, $J = 8.9, 16.2$ Hz), 2.83 (dd, 1 H, $J = 8.4, 13.0$ Hz), 2.92 (brs, 0.6 H), 3.29 (brs, 0.4 H), 3.83 (s, 1.8 H), 3.85 (s, 1.2 H), 4.26 (d, 0.4 H, $J = 13.0$ Hz), 4.28 (d, 0.6 H, $J = 13.0$ Hz), 4.95 (dd, 0.4 H, $J = 3.2, 8.9$ Hz), 5.10 (dd, 0.6 H, $J = 3.2, 9.7$ Hz), 5.22 (d, 0.4 H, $J = 8.4$ Hz), 5.24 (d, 0.6 H, $J = 8.4$ Hz), 6.82-6.86 (m, 1 H), 6.90-6.96 (m, 2 H), 7.06-7.36 (m, 1 H).

13c: R_f 0.36 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.72 (s, 1.5 H), 0.74 (s, 1.5 H), 0.760 (s, 1.5 H), 0.764 (s, 1.5 H), 1.01-1.12 (m, 1 H), 1.26 (s, 1.5 H), 1.28 (s, 1.5 H), 1.25-1.73 (m, 4 H), 1.89 (dd, 0.5 H, $J = 2.7, 16.7$ Hz), 1.91 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.18 (dd, 0.5 H, $J = 3.2, 16.7$ Hz), 2.28 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.74 (brs, 0.5 H), 2.83 (dd, 1 H, $J = 8.4, 13.0$ Hz), 3.38 (brs, 0.5 H), 3.80 (s, 3 H), 4.27 (d, 1 H, $J = 8.4$ Hz), 4.42 (dd, 0.5 H, $J = 2.7, 10.0$ Hz), 4.79 (dd, 0.5 H, $J = 3.2, 10.0$ Hz), 5.26 (d, 0.5 H, $J = 8.4$ Hz), 5.28 (d, 0.5 H, $J = 8.4$ Hz), 6.76-6.83 (m, 3 H), 7.09-7.32 (m, 11 H).

13d: R_f 0.34 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.73 (s, 3 H), 0.77 (s, 3 H), 1.02-1.12 (m, 1 H), 1.27 (s, 1.5 H), 1.28 (s, 1.5 H), 1.25-1.75 (m, 4 H), 1.87 (dd, 0.5 H, $J = 2.7, 16.7$ Hz), 1.92 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.14 (dd, 0.5 H, $J = 3.2, 16.7$ Hz), 2.28 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.68 (brs, 0.5 H), 2.83 (dd, 1 H, $J = 8.1, 13.0$ Hz), 3.30 (brs, 0.5 H), 3.79 (s, 3 H), 4.27 (d, 1 H, $J = 13.0$ Hz), 4.40 (dd, 0.5 H, $J = 2.7, 10.0$ Hz), 4.77 (dd, 0.5 H, $J = 3.2, 10.0$ Hz), 5.25 (d, 0.5 H, $J = 8.1$ Hz), 5.28 (d, 0.5 H, $J = 8.1$ Hz), 6.83-6.87 (m, 2 H), 7.05-7.28 (m, 12 H).

13e: R_f 0.34, 0.44 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.72 (s, 3 H), 0.76 (s, 3 H), 1.00-1.12 (m, 1 H), 1.27 (s, 3 H), 1.25-1.73 (m, 4 H), 1.84 (dd, 0.5 H, $J = 2.7, 16.7$ Hz), 1.88 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.14 (dd, 0.5 H, $J = 3.2, 16.7$ Hz), 2.26 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.83 (dd, 1 H, $J = 8.4, 13.2$ Hz), 2.85 (brs, 0.5 H), 3.48 (brs, 0.5 H), 4.27 (d, 1 H, $J = 13.2$ Hz), 4.41 (dd, 0.5 H, $J = 2.7, 10.0$ Hz), 4.78 (dd, 0.5 H, $J =$

3.2, 10.0 Hz), 5.25 (d, 0.5 H, $J = 8.4$ Hz), 5.28 (d, 0.5 H, $J = 8.4$ Hz), 6.95-7.03 (m, 2 H), 7.09-7.32 (m, 12 H).

13f: R_f 0.45 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.71 (s, 0.9 H), 0.73 (s, 2.1 H), 0.76 (s, 3 H), 1.00-1.15 (m, 1 H), 1.26 (s, 0.9 H), 1.28 (s, 2.1 H), 1.27-1.72 (m, 4 H), 1.989 (dd, 0.3 H, $J = 2.7, 16.7$ Hz), 1.993 (dd, 0.7 H, $J = 10.0, 16.7$ Hz), 2.24 (dd, 0.7 H, $J = 3.2, 16.7$ Hz), 2.37 (dd, 0.3 H, $J = 10.0, 16.7$ Hz), 2.83 (dd, 1 H, $J = 8.4, 13.0$ Hz), 2.90 (brs, 0.7 H), 3.50 (brs, 0.3 H), 4.27 (d, 1 H, $J = 13.0$ Hz), 4.62 (dd, 0.3 H, $J = 2.7, 10.0$ Hz), 4.99 (dd, 0.7 H, $J = 3.2, 10.0$ Hz), 5.28 (d, 0.7 H, $J = 8.4$ Hz), 5.30 (d, 0.3 H, $J = 8.4$ Hz), 7.09-7.50 (m, 13 H), 7.66-7.85 (m, 4 H).

13g: R_f 0.27, 0.33 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.72 (s, 1.5 H), 0.74 (s, 1.5 H), 0.76 (s, 3 H), 1.00-1.12 (m, 1 H), 1.28 (s, 1.5 H), 1.30 (s, 1.5 H), 1.27-1.73 (m, 4 H), 1.99 (dd, 0.5 H, $J = 3.2, 16.7$ Hz), 2.11 (dd, 0.5 H, $J = 9.2, 16.7$ Hz), 2.32 (dd, 0.5 H, $J = 3.5, 16.7$ Hz), 2.44 (dd, 0.5 H, $J = 9.2, 16.7$ Hz), 2.59 (brs, 0.5 H), 2.83 (dd, 1 H, $J = 8.1, 13.2$ Hz), 3.24 (brs, 0.5 H), 4.28 (d, 1 H, $J = 13.2$ Hz), 4.53 (dd, 0.5 H, $J = 3.2, 9.2$ Hz), 4.84 (dd, 0.5 H, $J = 3.5, 9.2$ Hz), 5.25 (d, 1 H, $J = 8.1$ Hz), 6.15 (t, 1 H, $J = 3.5$ Hz), 6.29 (dd, 1 H, $J = 1.8, 3.5$ Hz), 7.05-7.35 (m, 1 H).

13h: R_f 0.26, 0.30 (hexane-ethyl acetate, 5:1). ^1H NMR (CDCl_3) δ 0.74 (s, 3 H), 0.77 (s, 3 H), 1.00-1.13 (m, 1 H), 1.27 (s, 1.5 H), 1.28 (s, 1.5 H), 1.27-1.75 (m, 4 H), 1.84 (dd, 0.5 H, $J = 2.7, 16.7$ Hz), 1.88 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.12 (dd, 0.5 H, $J = 3.2, 16.7$ Hz), 2.26 (dd, 0.5 H, $J = 10.0, 16.7$ Hz), 2.72 (brs, 0.5 H), 2.82 (dd, 1 H, $J = 8.4, 13.0$ Hz), 3.34 (brs, 0.5 H), 4.26 (d, 1 H, $J = 13.0$ Hz), 4.34 (dd, 0.5 H, $J = 2.7, 10.0$ Hz), 4.72 (dd, 0.5 H, $J = 3.2, 10.0$ Hz), 5.25 (d, 0.5 H, $J = 8.4$ Hz), 5.28 (d, 0.5 H, $J = 8.4$ Hz), 5.93 (s, 2 H), 6.65-6.78 (m, 3 H), 7.10-7.32 (m, 10 H).

16a: R_f 0.75 (hexane-ethyl acetate, 5:1). $[\alpha]_D^{25} -62.5$ (c 1.2, CHCl_3). IR (KBr) 1732, 1599, 1495, 739, 700, 617 cm^{-1} . ^1H NMR (CDCl_3) δ 0.68 (s, 3 H), 0.74 (s, 3 H), 0.99-1.09 (m, 1 H), 1.28 (s, 3 H), 1.28-1.40 (m, 1 H), 1.44 (d, 1 H, $J = 3.8$ Hz), 1.45-1.70 (m, 2 H), 1.82-1.94 (m, 1 H), 2.00-2.13 (m, 1 H), 2.36-2.48 (m, 1 H), 2.56-2.68 (m, 1 H), 2.80 (dd, 1 H, $J = 8.4, 13.0$ Hz), 4.29 (d, 1 H, $J = 13.0$ Hz), 5.24 (d, 1 H, $J = 8.4$ Hz), 7.00-7.33 (m, 15 H). ^{13}C NMR (CDCl_3) δ 11.39 (q), 21.49 (q), 21.88 (q), 30.10 (t), 30.48 (t), 32.88 (t), 35.17 (t), 47.36 (s), 47.71 (d), 50.27 (s), 52.10 (s), 52.97 (d), 80.32 (d), 125.59 (d), 125.79 (d), 125.82 (d), 126.93 (d), 127.90 (d), 128.14 (d), 128.27 (d), 128.34 (d), 140.44 (s), 144.43 (s), 145.37 (s), 171.25 (s). Anal. Calcd for $\text{C}_{32}\text{H}_{36}\text{O}_2$: C,

84.91; H, 8.02. Found: C, 84.93; H, 8.01.

16b: *R_f* 0.68 (hexane-ethyl acetate, 5:1). $[\alpha]_{\text{D}}^{20}$ -56.9 (*c* 1.08, CHCl₃). IR (KBr) 1732, 1495, 746, 704, 617 cm⁻¹. ¹H NMR (CDCl₃) δ 0.70 (s, 3 H), 0.75 (s, 3 H), 1.00-1.12 (m, 1 H), 1.29 (s, 3 H), 1.30-1.70 (m, 4 H), 1.84-2.00 (m, 1 H), 2.01-2.15 (m, 1 H), 2.42-2.54 (m, 1 H), 2.60-2.72 (m, 1 H), 2.81 (dd, 1 H, *J* = 8.4, 13.0 Hz), 3.80 (s, 3 H), 4.29 (d, 1 H, *J* = 13.0 Hz), 5.21 (d, 1 H, *J* = 8.4 Hz), 6.78-6.86 (m, 2 H), 6.90-7.30 (m, 12 H). ¹³C NMR (CDCl₃) δ 11.40 (q), 20.90 (q), 21.88 (q), 25.53 (t), 30.11 (t), 32.83 (t), 33.60 (t), 47.34 (s), 47.70 (d), 50.24 (s), 52.11 (d), 53.00 (d), 54.95 (s), 80.02 (d), 109.92 (d), 120.14 (d), 125.55 (d), 125.74 (d), 126.89 (d), 127.12 (d), 127.89 (d), 128.20 (d), 128.31 (d), 128.79 (s), 129.44 (d), 144.36 (s), 145.40 (s), 157.06 (s), 171.59 (s). Anal. Calcd for C₃₃H₃₈O₃: C, 82.12; H, 7.94. Found: C, 82.01; H, 7.98.

16c: *R_f* 0.72 (hexane-ethyl acetate, 5:1). $[\alpha]_{\text{D}}^{20}$ -69.0 (*c* 0.96, CHCl₃). IR (KBr) 1732, 746, 696, 617 cm⁻¹. ¹H NMR (CDCl₃) δ 0.70 (s, 3 H), 0.75 (s, 3 H), 0.98-1.12 (m, 1 H), 1.28 (s, 3 H), 1.25-1.72 (m, 4 H), 1.80-1.95 (m, 1 H), 1.99-2.14 (m, 1 H), 2.33-2.46 (m, 1 H), 2.53-2.67 (m, 1 H), 2.81 (dd, 1 H, *J* = 8.4, 12.7 Hz), 3.77 (s, 3 H), 4.28 (d, 1 H, *J* = 12.7 Hz), 5.23 (d, 1 H, *J* = 8.4 Hz), 6.59-6.74 (m, 3 H), 7.05-7.31 (m, 11 H). ¹³C NMR (CDCl₃) δ 11.39 (q), 21.47 (q), 21.88 (q), 30.08 (t), 30.52 (t), 32.84 (t), 35.13 (t), 47.36 (s), 47.66 (d), 50.24 (s), 52.07 (d), 52.93 (d), 54.93 (q), 80.31 (d), 111.18 (d), 113.78 (d), 120.26 (d), 125.58 (d), 125.78 (d), 126.90 (d), 127.90 (d), 128.26 (d), 128.34 (d), 129.11 (d), 142.03 (s), 144.41 (s), 145.34 (s), 159.37 (s), 171.28 (s). Anal. Calcd for C₃₃H₃₈O₃: C, 82.12; H, 7.94. Found: C, 82.09; H, 7.92.

16d: *R_f* 0.67 (hexane-ethyl acetate, 5:1). mp 110-111 °C. $[\alpha]_{\text{D}}^{23}$ -67.5 (*c* 1.14, CHCl₃). IR (KBr) 1732, 1514, 748, 706, 617 cm⁻¹. ¹H NMR (CDCl₃) δ 0.69 (s, 3 H), 0.75 (s, 3 H), 1.00-1.10 (m, 1 H), 1.28 (s, 3 H), 1.33-1.70 (m, 4 H), 1.77-1.92 (m, 1 H), 1.97-2.10 (m, 1 H), 2.30-2.44 (m, 1 H), 2.50-2.63 (m, 1 H), 2.80 (dd, 1 H, *J* = 8.4, 13.0 Hz), 3.74 (s, 3 H), 4.29 (d, 1 H, *J* = 13.0 Hz), 5.23 (d, 1 H, *J* = 8.4 Hz), 6.76-6.82 (m, 2 H), 6.94-7.00 (m, 2 H), 7.04-7.16 (m, 2 H), 7.16-7.31 (m, 8 H). ¹³C NMR (CDCl₃) δ 11.47 (q), 21.55 (q), 21.96 (q), 29.70 (t), 30.19 (t), 32.93 (t), 35.58 (t), 47.46 (s), 47.78 (d), 50.35 (s), 52.17 (d), 53.03 (d), 55.23 (q), 80.37 (d), 113.70 (d), 125.68 (d), 125.87 (d), 126.99 (d), 128.00 (d), 128.36 (d), 128.43 (d), 128.91 (d), 132.64 (s), 144.51 (s), 145.46 (s), 157.76 (s), 171.51 (s). Anal. Calcd for C₃₃H₃₈O₃: C, 82.12; H, 7.94. Found: C, 82.01; H, 7.98.

16e: *R*_f 0.64 (hexane-ethyl acetate, 5:1). $[\alpha]_{\text{D}}^{23}$ -72.1 (*c* 0.92, CHCl₃). IR (KBr) 1732, 1495, 746, 617 cm⁻¹. ¹H NMR (CDCl₃) δ 0.67 (s, 3 H), 0.75 (s, 3 H), 1.00-1.10 (m, 1 H), 1.27 (s, 3 H), 1.30-1.70 (m, 4 H), 1.77-1.89 (m, 1 H), 1.98-2.10 (m, 1 H), 2.34-2.47 (m, 1 H), 2.52-2.65 (m, 1 H), 2.80 (dd, 1 H, *J* = 8.1, 13.0 Hz), 4.28 (d, 1 H, *J* = 13.0 Hz), 5.22 (d, 1 H, *J* = 8.1 Hz), 6.89-7.04 (m, 4 H), 7.04-7.30 (m, 10 H). ¹³C NMR (CDCl₃) δ 11.39 (q), 21.50 (q), 21.88 (q), 29.64 (t), 30.10 (t), 32.87 (t), 35.21 (t), 47.39 (s), 47.69 (d), 50.27 (s), 52.10 (d), 52.93 (d), 80.43 (d), 114.90 (d, *J*_{CCF} = 21.1 Hz), 125.60 (d), 125.83 (d), 126.93 (d), 127.93 (d), 128.27 (d), 128.38 (d), 129.35 (d, *J*_{CCCF} = 7.7 Hz), 136.10 (s, *J*_{CCCF} = 3.4 Hz), 144.48 (s), 145.35 (s), 161.11 (s, *J*_{CF} = 241.6 Hz), 171.18 (s). Anal. Calcd for C₃₂H₃₅FO₂: C, 81.67; H, 7.50. Found: C, 81.55; H, 7.58.

16f: *R*_f 0.47 (hexane-ethyl acetate, 5:1). mp 45-47 °C. $[\alpha]_{\text{D}}^{20}$ -56.6 (*c* 1.08, CHCl₃). IR (KBr) 1734, 1494, 745, 702, 617 cm⁻¹. ¹H NMR (CDCl₃) δ 0.67 (s, 3 H), 0.72 (s, 3 H), 0.98-1.08 (m, 1 H), 1.28 (s, 3 H), 1.30-1.68 (m, 4 H), 1.88-2.01 (m, 1 H), 2.09-2.22 (m, 1 H), 2.52-2.65 (m, 1 H), 2.72-2.85 (m, 2 H), 4.29 (d, 1 H, *J* = 13.2 Hz), 5.25 (d, 1 H, *J* = 8.4 Hz), 7.03-7.13 (m, 2 H), 7.15-7.45 (m, 11 H), 7.57 (brs, 1 H), 7.68-7.77 (m, 3 H). ¹³C NMR (CDCl₃) δ 11.36 (q), 21.47 (q), 21.82 (q), 30.02 (t), 30.57 (t), 32.81 (t), 35.02 (t), 47.29 (s), 47.62 (d), 50.19 (s), 52.03 (d), 52.88 (d), 80.30 (d), 124.98 (d), 125.54 (d), 125.66 (d), 125.75 (d), 125.99 (d), 126.63 (d), 126.87 (d), 127.15 (d), 127.30 (s), 127.69 (d), 127.86 (d), 128.23 (d), 128.30 (d), 131.82 (s), 133.30 (s), 137.90 (s), 144.38 (s), 145.31 (s), 171.20 (s). Anal. Calcd for C₃₆H₃₈O₂: C, 86.02; H, 7.62. Found: C, 85.87; H, 7.70.

16g: *R*_f 0.70 (hexane-ethyl acetate, 5:1). mp 97-98 °C. $[\alpha]_{\text{D}}^{20}$ -62.1 (*c* 1.07, CHCl₃). IR (KBr) 1738, 1493, 1481, 741, 706, 619 cm⁻¹. ¹H NMR (CDCl₃) δ 0.71 (s, 3 H), 0.75 (s, 3 H), 1.00-1.10 (m, 1 H), 1.29 (s, 3 H), 1.25-1.71 (m, 4 H), 1.85-1.98 (m, 1 H), 2.02-2.15 (m, 1 H), 2.40-2.53 (m, 1 H), 2.58-2.71 (m, 1 H), 2.81 (dd, 1 H, *J* = 8.1, 13.0 Hz), 4.28 (d, 1 H, *J* = 13.0 Hz), 5.22 (d, 1 H, *J* = 8.1 Hz), 5.88 (d, 1 H, *J* = 3.0 Hz), 6.23 (dd, 1 H, *J* = 1.9, 3.0 Hz), 7.04-7.15 (m, 2 H), 7.17-7.30 (m, 9 H). ¹³C NMR (CDCl₃) δ 11.37 (q), 21.47 (q), 21.86 (q), 23.02 (t), 30.07 (t), 31.91 (t), 32.83 (t), 47.35 (s), 47.63 (d), 50.24 (s), 52.07 (d), 52.93 (d), 80.41 (d), 104.80 (d), 109.89 (d), 125.58 (d), 125.78 (d), 126.85 (d), 127.87 (d), 128.25 (d), 128.33 (d), 140.69 (d), 144.32 (s), 145.26 (s), 153.98 (s), 170.85 (s). Anal. Calcd for C₃₀H₃₄O₃: C, 81.41; H, 7.74. Found: C, 81.49; H, 7.80.

16h: *R_f* 0.67 (hexane-ethyl acetate, 5:1). $[\alpha]_D^{24}$ -70.5 (*c* 5.6, CHCl₃). IR (KBr) 1732, 1491, 758, 704, 617 cm⁻¹. ¹H NMR (CDCl₃) δ 0.69 (s, 3 H), 0.75 (s, 3 H), 1.00 -1.10 (m, 1 H), 1.28 (s, 3 H), 1.29-1.72 (m, 4 H), 1.75-1.88 (m, 1 H), 1.95-2.09 (m, 1 H), 2.26-2.40 (m, 1 H), 2.47-2.60 (m, 1 H), 2.80 (dd, 1 H, *J* = 8.1, 13.0 Hz), 4.28 (d, 1 H, *J* = 13.0 Hz), 5.22 (d, 1 H, *J* = 8.1 Hz), 5.88 (s, 2 H), 6.47-6.55 (m, 2 H), 6.68 (d, 1 H, *J* = 7.8 Hz), 7.05-7.30 (m, 10 H). ¹³C NMR (CDCl₃) δ 11.45 (q), 21.54 (q), 21.94 (q), 30.16 (t), 30.28 (t), 32.90 (t), 35.55 (t), 47.45 (s), 47.73 (d), 50.32 (s), 52.13 (d), 52.98 (d), 80.39 (d), 100.65 (t), 108.01 (d), 108.55 (d), 120.75 (d), 125.66 (d), 125.86 (d), 126.96 (d), 127.98 (d), 128.34 (d), 128.41 (d), 134.35 (s), 144.48 (s), 145.41 (s), 145.59 (s), 147.34 (s), 171.35 (s). Anal. Calcd for C₃₃H₃₆O₄: C, 79.81; H, 7.31. Found: C, 79.80; H, 7.37.

References

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Results of Calculations

Optimized Structures of Transition States for the hydrocoupling of 1a

dl-TS (UHF/AM1)

Z-Matrix orientation:

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O 0 -3.239395 -1.780319 -2.402039  
C 0 0.772430 0.741547 -1.441772  
C 0 0.233994 1.950043 -1.938950  
C 0 1.057251 3.019821 -2.277847  
C 0 2.444458 2.924728 -2.129257  
C 0 2.996536 1.741684 -1.626266  
C 0 2.179565 0.667862 -1.288925  
C 0 -0.047043 -0.405014 -1.102371  
C 0 -1.407822 -0.464828 -1.543793  
C 0 -2.047150 -1.600143 -2.022079  
O 0 -1.248627 -2.759262 -2.147400  
C 0 -1.913100 -3.927231 -2.568451  
H 0 -0.855148 2.037430 -2.061371  
H 0 0.614868 3.948151 -2.664719  
H 0 3.090851 3.768723 -2.398148  
H 0 4.084290 1.663116 -1.492400  
H 0 2.612305 -0.252151 -0.863907  
H 0 0.502823 -1.370209 -1.147812  
H 0 -2.028214 0.436462 -1.486557  
H 0 -2.302963 -3.809982 -3.610306  
H 0 -2.765381 -4.173248 -1.888382  
H 0 -1.133972 -4.730179 -2.530411  
O 0 3.109879 -1.941315 2.157852  
C 0 -0.042236 -0.436859 0.903885  
C 0 -0.829483 0.720886 1.279800  
C 0 -0.257690 1.897507 1.814621  
C 0 -1.050919 2.978622 2.187576  
C 0 -2.440200 2.927063 2.036758  
C 0 -3.024887 1.776382 1.496887  
C 0 -2.238083 0.691345 1.125351  
C 0 1.316193 -0.548584 1.342606  
C 0 1.923386 -1.715973 1.784317  
O 0 1.092743 -2.855728 1.873093  
C 0 1.724152 -4.054626 2.256531  
H 0 -0.618820 -1.387268 0.918991  
H 0 0.833359 1.950546 1.939178  
H 0 -0.582900 3.881531 2.603348  
H 0 -3.062759 3.779861 2.332520  
H 0 -4.114304 1.732468 1.361191  
H 0 -2.696198 -0.202271 0.671646  
H 0 1.961533 0.336380 1.313736  
H 0 2.116714 -3.981415 3.301407
```

H 0	2.569550	-4.302582	1.568604
H 0	0.922943	-4.833847	2.193344

 SCF Energy: -0.12608 hartrees (-79.12 kcal/mole)
 Only One Imaginary Frequency: -896.1509

Optimized Structures of Transition States for the hydrocoupling of 1a
meso-TS (UHF/AM1)

Z-Matrix orientation:

C 0	-0.877594	1.340042	1.913300
C 0	-0.705688	2.682526	2.320694
C 0	-1.794693	3.468506	2.688538
C 0	-3.089340	2.943802	2.650192
C 0	-3.281219	1.625900	2.220459
C 0	-2.196869	0.835342	1.853256
C 0	0.274963	0.532776	1.564377
C 0	0.308044	-0.848100	1.944824
C 0	1.499756	-1.502182	2.220886
O 0	2.711609	-1.150238	2.232300
O 0	1.321167	-2.860428	2.605286
C 0	2.497971	-3.591064	2.850388
H 0	0.308029	3.106918	2.343262
H 0	-1.636856	4.507370	3.009033
H 0	-3.947021	3.562531	2.940720
H 0	-4.299561	1.218185	2.158798
H 0	-2.350479	-0.187241	1.477203
H 0	1.244797	1.057770	1.703308
H 0	-0.623032	-1.420471	1.971176
H 0	3.175491	-3.574814	1.961288
H 0	3.047852	-3.177292	3.732361
H 0	2.153061	-4.635345	3.062546
C 0	0.247589	0.538788	-0.457916
C 0	1.359421	1.440353	-0.703766
C 0	2.672638	1.072021	-0.314713
C 0	3.751236	1.915329	-0.554642
C 0	3.563644	3.154175	-1.179703
C 0	2.273361	3.539871	-1.555450
C 0	1.188202	2.699524	-1.321243
C 0	-1.044907	0.868958	-0.980637
C 0	-1.817215	-0.032623	-1.698990
O 0	-1.650818	-1.206970	-2.119385
O 0	-3.076400	0.509521	-2.094788
C 0	-3.914215	-0.347382	-2.829666
H 0	0.515411	-0.537476	-0.515152
H 0	2.815689	0.114670	0.221176
H 0	4.760147	1.610900	-0.243546

H 0	4.417725	3.815582	-1.367935
H 0	2.116989	4.511932	-2.042908
H 0	0.176712	3.002289	-1.629669
H 0	-1.462189	1.860123	-0.778458
H 0	-3.447723	-0.620453	-3.809006
H 0	-4.132446	-1.284363	-2.260025
H 0	-4.855164	0.236816	-2.997482

SCF Energy: -0.12136 hartrees (-76.15 kcal/mole)

Only One Imaginary Frequency: -893.5390

Optimized Structures of Transition States for the hydrocoupling of 1a

dl-TS (UHF/PM3)

Z-Matrix orientation:

C 0	0.559067	0.994980	-1.488068
C 0	1.918854	1.296265	-1.251297
C 0	2.464218	2.498520	-1.676331
C 0	1.675323	3.441925	-2.337662
C 0	0.319229	3.178619	-2.539993
C 0	-0.233215	1.979355	-2.116882
C 0	0.008774	-0.290665	-1.096481
C 0	-1.337234	-0.589752	-1.491974
C 0	-1.836639	-1.828751	-1.891495
O 0	-3.007233	-2.147675	-2.203354
O 0	-0.900345	-2.868332	-2.014679
C 0	-1.380600	-4.153992	-2.279037
H 0	2.509506	0.579346	-0.655426
H 0	3.518829	2.715179	-1.483887
H 0	2.110992	4.384064	-2.678116
H 0	-0.309570	3.924957	-3.033478
H 0	-1.302185	1.754013	-2.253998
H 0	0.736359	-1.119019	-1.125031
H 0	-2.057053	0.241180	-1.443466
H 0	-1.842255	-4.236710	-3.271088
H 0	-2.097107	-4.505981	-1.527298
H 0	-0.479584	-4.774918	-2.245865
C 0	0.058502	-0.271545	0.973892
C 0	-0.566269	0.977402	1.380203
C 0	-1.908447	1.245438	1.027847
C 0	-2.541260	2.401886	1.457794
C 0	-1.860336	3.333008	2.244232
C 0	-0.525009	3.099777	2.574203
C 0	0.115463	1.944900	2.147064
C 0	1.425705	-0.515198	1.343674
C 0	1.934448	-1.683777	1.905487
O 0	3.119202	-1.983719	2.183517

O 0	0.991013	-2.660538	2.272339
C 0	1.468246	-3.900314	2.705521
H 0	-0.628479	-1.133804	1.022476
H 0	-2.411545	0.540054	0.342102
H 0	-3.579712	2.591690	1.171524
H 0	-2.363678	4.240082	2.586517
H 0	0.019165	3.833466	3.175766
H 0	1.163742	1.757767	2.411179
H 0	2.158890	0.260483	1.087296
H 0	2.006668	-3.836029	3.659607
H 0	2.115600	-4.391281	1.969086
H 0	0.557251	-4.491700	2.843918

SCF Energy: -0.11821 hartrees (-74.18 kcal/mole)
Only One Imaginary Frequency: -819.9821

Optimized Structures of Transition States for the hydrocoupling of 1a
meso-TS (UHF/PM3)

Z-Matrix orientation:

C 0	2.426086	-2.634415	-2.190857
C 0	3.650238	-1.986191	-2.002533
C 0	3.683655	-0.682648	-1.501587
C 0	2.497910	-0.019470	-1.178711
C 0	1.248795	-0.644760	-1.343735
C 0	1.231171	-1.972153	-1.867844
C 0	0.000809	0.001144	-1.002640
C 0	-1.181213	-0.673203	-1.459900
C 0	-1.167480	-1.962158	-1.960266
O 0	0.074890	-2.666718	-2.099731
O 0	-2.069397	-2.733841	-2.376800
H 0	2.385147	-3.654922	-2.590179
H 0	4.584213	-2.506546	-2.250839
H 0	4.647247	-0.178207	-1.351517
H 0	2.523895	0.996353	-0.754791
H 0	-0.001800	1.105606	-1.050354
H 0	-2.143127	-0.160721	-1.381546
C 0	-2.497849	0.019516	1.178711
C 0	-3.683670	0.682648	1.501587
C 0	-3.650300	1.986145	2.002548
C 0	-2.426102	2.634384	2.190903
C 0	-1.231186	1.972153	1.867859
C 0	-1.248749	0.644760	1.343704
O 0	-0.074905	2.666733	2.099777
C 0	1.167511	1.962219	1.960251
C 0	1.181213	0.673248	1.459885
C 0	-0.000809	-0.001100	1.002579

O 0	2.069351	2.733871	2.376816
H 0	-2.523865	-0.996307	0.754700
H 0	-4.647232	0.178192	1.351500
H 0	-4.584213	2.506516	2.250870
H 0	-2.385132	3.654892	2.590302
H 0	2.143127	0.160721	1.381516
H 0	0.001800	-1.105591	1.050308

 SCF Energy: -0.09457 hartrees (-59.34 kcal/mole)

Only One Imaginary Frequency: -971.6404

Optimized Structures of Transition States for the hydrocoupling of 9

dl-TS (UHF/AM1)

Z-Matrix orientation:

C 0	-0.237167	1.803864	-2.779633
C 0	1.025452	2.352432	-2.539719
C 0	1.971268	1.641403	-1.796112
C 0	1.664230	0.377441	-1.289902
C 0	0.405960	-0.207900	-1.517242
C 0	-0.551361	0.532500	-2.272034
C 0	0.064102	-1.524567	-1.029007
C 0	-1.215317	-2.028534	-1.446335
C 0	-2.129578	-1.274139	-2.157440
O 0	-1.802597	0.059479	-2.566040
O 0	-3.284592	-1.516708	-2.595123
H 0	-0.989990	2.354004	-3.356934
H 0	1.268234	3.348373	-2.932129
H 0	2.955658	2.083984	-1.595169
H 0	2.389877	-0.170242	-0.667679
H 0	0.899857	-2.252426	-1.024139
H 0	-1.495850	-3.046005	-1.164902
C 0	-1.688461	0.204956	1.297272
C 0	-2.099213	1.425781	1.834854
C 0	-1.214996	2.194122	2.597153
C 0	0.089127	1.746689	2.824478
C 0	0.507507	0.519058	2.285294
C 0	-0.385635	-0.279100	1.511093
O 0	1.794083	0.144577	2.568604
C 0	2.230545	-1.146439	2.126846
C 0	1.381454	-1.956131	1.395996
C 0	0.064148	-1.550064	0.990173
O 0	3.402191	-1.302994	2.559509
H 0	-2.366745	-0.385376	0.660690
H 0	-3.117233	1.789841	1.644135
H 0	-1.539444	3.156189	3.014297
H 0	0.794189	2.342819	3.416229

H 0 1.745453 -2.939300 1.089310
H 0 -0.708145 -2.344635 0.966064

SCF Energy: -0.09045 hartrees (--56.76 kcal/mole)
Only One Imaginary Frequency: -939.7294

Optimized Structures of Transition States for the hydrocoupling of 9
meso-TS (UHF/AM1)

Z-Matrix orientation:

C 0 -0.877594 1.340042 1.913300
C 0 -0.705688 2.682526 2.320694
C 0 -1.794693 3.468506 2.688538
C 0 -3.089340 2.943802 2.650192
C 0 -3.281219 1.625900 2.220459
C 0 -2.196869 0.835342 1.853256
C 0 0.274963 0.532776 1.564377
C 0 0.308044 -0.848100 1.944824
C 0 1.499756 -1.502182 2.220886
O 0 2.711609 -1.150238 2.232300
O 0 1.321167 -2.860428 2.605286
C 0 2.497971 -3.591064 2.850388
H 0 0.308029 3.106918 2.343262
H 0 -1.636856 4.507370 3.009033
H 0 -3.947021 3.562531 2.940720
H 0 -4.299561 1.218185 2.158798
H 0 -2.350479 -0.187241 1.477203
H 0 1.244797 1.057770 1.703308
H 0 -0.623032 -1.420471 1.971176
H 0 3.175491 -3.574814 1.961288
H 0 3.047852 -3.177292 3.732361
H 0 2.153061 -4.635345 3.062546
C 0 0.247589 0.538788 -0.457916
C 0 1.359421 1.440353 -0.703766
C 0 2.672638 1.072021 -0.314713
C 0 3.751236 1.915329 -0.554642
C 0 3.563644 3.154175 -1.179703
C 0 2.273361 3.539871 -1.555450
C 0 1.188202 2.699524 -1.321243
C 0 -1.044907 0.868958 -0.980637
C 0 -1.817215 -0.032623 -1.698990
O 0 -1.650818 -1.206970 -2.119385
O 0 -3.076400 0.509521 -2.094788
C 0 -3.914215 -0.347382 -2.829666
H 0 0.515411 -0.537476 -0.515152
H 0 2.815689 0.114670 0.221176
H 0 4.760147 1.610900 -0.243546

H 0	4.417725	3.815582	-1.367935
H 0	2.116989	4.511932	-2.042908
H 0	0.176712	3.002289	-1.629669
H 0	-1.462189	1.860123	-0.778458
H 0	-3.447723	-0.620453	-3.809006
H 0	-4.132446	-1.284363	-2.260025
H 0	-4.855164	0.236816	-2.997482

 SCF Energy: -0.12136 hartrees (-76.15 kcal/mole)

Only One Imaginary Frequency: -893.5390

Optimized Structures of Transition States for the hydrocoupling of 9

dl-TS (UHF/PM3)

Z-Matrix orientation:

C 0	0.123215	1.735855	2.820206
C 0	-1.156067	2.232864	2.562683
C 0	-2.054596	1.495331	1.793854
C 0	-1.688614	0.255554	1.274994
C 0	-0.410675	-0.274094	1.514069
C 0	0.497864	0.491287	2.300323
C 0	-0.008194	-1.563766	0.996719
C 0	1.268631	-2.041626	1.461000
C 0	2.122162	-1.239059	2.204132
O 0	1.758316	0.057922	2.615067
O 0	3.259140	-1.407135	2.687393
H 0	0.827805	2.317719	3.421051
H 0	-1.447632	3.208298	2.960388
H 0	-3.048538	1.898376	1.582016
H 0	-2.378571	-0.311508	0.637772
H 0	-0.815109	-2.314865	0.941559
H 0	1.587341	-3.045334	1.185120
C 0	1.674713	0.379654	-1.262360
C 0	1.985641	1.653915	-1.731186
C 0	1.055054	2.381393	-2.470886
C 0	-0.201462	1.839569	-2.749069
C 0	-0.520813	0.560104	-2.279388
C 0	0.420929	-0.195419	-1.523453
O 0	-1.761414	0.084946	-2.612213
C 0	-2.067871	-1.242065	-2.253479
C 0	-1.179443	-2.035461	-1.542084
C 0	0.075729	-1.521057	-1.058090
O 0	-3.196793	-1.440445	-2.744034
H 0	2.389297	-0.181610	-0.647598
H 0	2.961258	2.091339	-1.502625
H 0	1.303375	3.383682	-2.829193
H 0	-0.931351	2.413467	-3.326904

H 0 -1.453690 -3.062332 -1.306656
H 0 0.914749 -2.237732 -1.032120

SCF Energy: -0.11719 hartrees (-73.54 kcal/mole)
Only One Imaginary Frequency: -939.6257

Optimized Structures of Transition States for the hydrocoupling of 9
meso-TS (UHF/PM3)

Z-Matrix orientation:

C 0 2.410950 -2.648621 -2.233246
C 0 3.633270 -1.994156 -2.064590
C 0 3.667603 -0.689926 -1.576523
C 0 2.487503 -0.027771 -1.243912
C 0 1.241989 -0.660233 -1.385086
C 0 1.222641 -1.988647 -1.900925
C 0 -0.000870 -0.009857 -1.022980
C 0 -1.187607 -0.678802 -1.485657
C 0 -1.149841 -1.979065 -1.969971
O 0 0.063202 -2.681107 -2.123718
O 0 -2.016968 -2.776917 -2.374695
H 0 2.384460 -3.669250 -2.625229
H 0 4.563004 -2.510056 -2.317612
H 0 4.627502 -0.184021 -1.442520
H 0 2.515274 0.985931 -0.824905
H 0 -0.001358 1.089905 -1.084091
H 0 -2.146927 -0.169678 -1.400436
C 0 -2.495193 0.035934 1.244522
C 0 -3.671814 0.705093 1.575500
C 0 -3.630539 2.009689 2.061935
C 0 -2.404663 2.657486 2.230835
C 0 -1.219833 1.990509 1.900085
C 0 -1.246246 0.661667 1.385483
O 0 -0.056747 2.676559 2.123154
C 0 1.152481 1.967500 1.971237
C 0 1.183304 0.666687 1.487793
C 0 -0.006775 0.004318 1.024338
O 0 2.023651 2.760712 2.376358
H 0 -2.528366 -0.978333 0.827393
H 0 -4.634460 0.204391 1.441574
H 0 -4.557495 2.531204 2.313583
H 0 -2.372665 3.678284 2.621826
H 0 2.139786 0.152237 1.403168
H 0 -0.012390 -1.095413 1.085266

SCF Energy: -0.12006 hartrees (-75.34 kcal/mole)
Only One Imaginary Frequency: -894.9083

Optimized Structures of Anion Radical of 14a

A by UHF/AM1

Z-Matrix orientation:

```
-----  
C 0 -2.946625  0.066956  0.903442  
C 0 -4.206329 -0.448151  0.162964  
C 0 -4.174225  0.296829 -1.182205  
C 0 -2.898010  1.164139 -1.086487  
C 0 -1.720016  0.168152 -1.231705  
C 0 -1.747757 -0.591049  0.139450  
C 0 -2.886154  1.555954  0.425200  
C 0 -2.944733 -0.175400  2.376770  
O 0 -0.528992 -0.435196  0.834671  
C 0 -1.649033  2.320786  0.850021  
C 0 -4.092422  2.378815  0.835007  
C 0 -0.369263  0.772476 -1.612213  
C 0 -0.060715 -1.510773  1.616409  
C 0  0.536530 -0.282898 -2.192841  
C 0 -0.466660  1.943130 -2.548126  
C 0  0.346390  3.062347 -2.316437  
C 0  0.307190  4.158798 -3.175842  
C 0 -0.546600  4.156464 -4.278046  
C 0 -1.364807  3.052307 -4.513123  
C 0 -1.326447  1.955032 -3.654587  
C 0  0.430298 -0.699707 -3.524551  
C 0  1.293655 -1.667038 -4.036300  
C 0  2.270798 -2.235764 -3.221039  
C 0  2.374619 -1.837616 -1.888748  
C 0  1.513489 -0.868683 -1.375809  
C 0  1.197281 -1.231659  2.201492  
O 0 -0.813431 -2.504364  1.661804  
C 0  1.844894 -2.168045  2.998047  
C 0  3.087600 -2.000610  3.628067  
C 0  3.633270 -3.061523  4.412888  
C 0  4.858704 -2.932663  5.047974  
C 0  5.600600 -1.747131  4.935684  
C 0  5.085495 -0.689789  4.170959  
C 0  3.860550 -0.807693  3.531219  
H 0 -4.165512 -1.554443  0.023132  
H 0 -5.129715 -0.208740  0.742050  
H 0 -5.079407  0.933929 -1.323288  
H 0 -4.124756 -0.412155 -2.042679  
H 0 -2.879288  2.022461 -1.783890  
H 0 -1.978561 -0.576370 -2.035416  
H 0 -1.957062 -1.682510 -0.030334  
H 0 -2.089310  0.369308  2.848358
```

H 0	-2.810913	-1.268066	2.579697
H 0	-3.898560	0.176147	2.838913
H 0	-0.844452	1.635773	1.213608
H 0	-1.885132	3.027679	1.683792
H 0	-1.253891	2.915680	-0.010529
H 0	-4.010330	3.406540	0.403534
H 0	-4.125809	2.459686	1.949692
H 0	-5.058411	1.938309	0.496323
H 0	0.112411	1.141571	-0.654816
H 0	1.022110	3.072479	-1.447281
H 0	0.952805	5.027542	-2.982315
H 0	-0.575912	5.020264	-4.956314
H 0	-2.043884	3.045746	-5.377686
H 0	-1.987366	1.093552	-3.837418
H 0	-0.336960	-0.261627	-4.179245
H 0	1.199554	-1.982269	-5.084824
H 0	2.950256	-2.999466	-3.623947
H 0	3.128250	-2.294739	-1.229919
H 0	1.574234	-0.592041	-0.305800
H 0	1.630768	-0.244034	2.011642
H 0	1.334351	-3.136307	3.146835
H 0	3.059738	-3.993805	4.507202
H 0	5.257462	-3.763748	5.646423
H 0	6.569183	-1.648636	5.438812
H 0	5.663254	0.240891	4.081039
H 0	3.470444	0.029907	2.937485

SCF Energy: -0.05295 hartrees (-33.23 kcal/mole)
Vibration analysis showed no imaginary frequency.

Optimized Structures of Anion Radical of 14a

B by UHF/AM1

Z-Matrix orientation:

C 0	-1.862534	0.746323	1.077393
C 0	-3.125946	0.232620	0.341202
C 0	-3.132324	1.018982	-0.979736
C 0	-1.862915	1.895432	-0.885376
C 0	-0.677811	0.918961	-1.078018
C 0	-0.664398	0.124329	0.278458
C 0	-1.825623	2.248291	0.635147
C 0	-1.861130	0.482025	2.547546
O 0	0.567657	0.286255	0.940811
C 0	-0.587387	3.014374	1.055237
C 0	-3.032898	3.054123	1.075531
C 0	0.657715	1.549133	-1.470337
C 0	1.125229	-0.795273	1.659409

C 0	1.557434	0.525848	-2.114059
C 0	0.529480	2.753433	-2.358902
C 0	1.334854	3.872086	-2.098984
C 0	1.269760	4.999527	-2.915604
C 0	0.397186	5.029251	-4.002625
C 0	-0.413559	3.925919	-4.265381
C 0	-0.349213	2.797714	-3.449493
C 0	1.403778	0.139694	-3.450256
C 0	2.263779	-0.796783	-4.021744
C 0	3.284851	-1.364731	-3.261627
C 0	3.435425	-0.997055	-1.925110
C 0	2.578171	-0.059052	-1.351273
C 0	0.348419	-1.903961	2.055862
O 0	2.330368	-0.522293	1.852844
C 0	0.922348	-2.981354	2.724091
C 0	0.250061	-4.122650	3.187302
C 0	0.982040	-5.157318	3.845612
C 0	0.352829	-6.299561	4.315796
C 0	-1.030700	-6.470291	4.156616
C 0	-1.772446	-5.467560	3.514557
C 0	-1.153183	-4.320496	3.040192
H 0	-3.067963	-0.868103	0.165955
H 0	-4.042160	0.434784	0.945206
H 0	-4.046036	1.652084	-1.078232
H 0	-3.096802	0.338211	-1.863327
H 0	-1.867645	2.772934	-1.559143
H 0	-0.943848	0.189529	-1.892838
H 0	-0.859955	-0.960159	0.064392
H 0	-0.832443	0.633286	2.961639
H 0	-2.168671	-0.572433	2.755981
H 0	-2.570648	1.169067	3.069946
H 0	0.217651	2.328964	1.417800
H 0	-0.820145	3.724609	1.886993
H 0	-0.193802	3.607407	0.192490
H 0	-3.003174	4.061691	0.592758
H 0	-3.013672	3.190979	2.185028
H 0	-4.001100	2.570100	0.810303
H 0	1.161209	1.884964	-0.511093
H 0	2.025360	3.856491	-1.241500
H 0	1.909378	5.867432	-2.700287
H 0	0.347412	5.917465	-4.647369
H 0	-1.107239	3.944305	-5.118011
H 0	-1.004868	1.936920	-3.653610
H 0	0.601028	0.576965	-4.061478
H 0	2.131805	-1.089020	-5.072800
H 0	3.960770	-2.105362	-3.710876
H 0	4.222885	-1.456543	-1.309600
H 0	2.674362	0.190781	-0.275330

H 0	-0.726379	-1.896317	1.849213
H 0	2.010864	-2.932419	2.906708
H 0	2.065933	-5.032806	3.975296
H 0	0.938385	-7.081970	4.818710
H 0	-1.524963	-7.374741	4.529144
H 0	-2.856644	-5.596878	3.388702
H 0	-1.749542	-3.544174	2.542191

 SCF Energy: -0.04798 hartrees (-30.11 kcal/mole)
 Vibration analysis showed no imaginary frequency.

Optimized Structures of Anion Radical of 14a

A by UB3LYP/3-21G*

Z-Matrix orientation:

C 0	-3.685989	-0.414230	0.603531
C 0	-4.874283	-1.110229	-0.133087
C 0	-4.867966	-0.452240	-1.563293
C 0	-3.631210	0.497131	-1.492294
C 0	-2.395523	-0.473984	-1.516647
C 0	-2.405350	-1.051163	-0.036835
C 0	-3.709595	1.025436	-0.022095
C 0	-3.714767	-0.538742	2.124908
O 0	-1.189850	-0.698776	0.687347
C 0	-2.519104	1.917923	0.402557
C 0	-5.005463	1.819260	0.264969
C 0	-1.007004	0.096664	-1.971786
C 0	-0.730820	-1.740906	1.654648
C 0	-0.104370	-1.061508	-2.461258
C 0	-1.100479	1.188339	-3.033707
C 0	-0.267502	2.312271	-2.935913
C 0	-0.286880	3.316147	-3.906647
C 0	-1.145706	3.215103	-5.002747
C 0	-1.984848	2.103592	-5.114639
C 0	-1.963211	1.103577	-4.140106
C 0	0.014526	-1.402847	-3.816467
C 0	0.817184	-2.472870	-4.220490
C 0	1.523956	-3.218857	-3.275940
C 0	1.419296	-2.882797	-1.924423
C 0	0.613312	-1.817490	-1.520386
C 0	0.512772	-1.371994	2.190735
O 0	-1.459747	-2.740204	1.847122
C 0	1.172470	-2.198700	3.109756
C 0	2.434189	-1.979904	3.726318
C 0	2.966949	-2.936722	4.650620
C 0	4.195374	-2.758545	5.264923
C 0	4.977356	-1.618149	5.002243

C 0	4.479782	-0.662354	4.099594
C 0	3.251465	-0.827835	3.478271
H 0	-4.723557	-2.194321	-0.171616
H 0	-5.817032	-0.916733	0.389557
H 0	-5.791306	0.104889	-1.750366
H 0	-4.753387	-1.195343	-2.359421
H 0	-3.616608	1.271530	-2.258743
H 0	-2.628876	-1.297821	-2.200455
H 0	-2.491730	-2.139923	-0.006866
H 0	-2.926041	0.080795	2.562714
H 0	-3.502625	-1.574097	2.408981
H 0	-4.685532	-0.224228	2.528183
H 0	-1.613983	1.324783	0.515167
H 0	-2.735458	2.379089	1.374954
H 0	-2.366791	2.721436	-0.328903
H 0	-4.990906	2.763260	-0.296173
H 0	-5.055786	2.063034	1.333038
H 0	-5.913757	1.274277	-0.002441
H 0	-0.520966	0.519577	-1.092316
H 0	0.404190	2.393402	-2.088150
H 0	0.366974	4.175659	-3.805435
H 0	-1.164612	3.993027	-5.758011
H 0	-2.660324	2.016693	-5.959122
H 0	-2.627853	0.251816	-4.231766
H 0	-0.500061	-0.813263	-4.564072
H 0	0.895462	-2.715027	-5.275665
H 0	2.150864	-4.046982	-3.588974
H 0	1.961838	-3.446655	-1.173843
H 0	0.524445	-1.577408	-0.470642
H 0	0.927017	-0.427673	1.862671
H 0	0.650818	-3.117615	3.371490
H 0	2.377000	-3.823914	4.864227
H 0	4.560059	-3.511383	5.959122
H 0	5.939575	-1.480942	5.483200
H 0	5.069321	0.224900	3.882324
H 0	2.895615	-0.073990	2.784943

SCF Energy: -1382.75655 hartrees

Optimized Structures of Anion Radical of 14a

B by UB3LYP/3-21G*

Z-Matrix orientation:

C 0	-2.410873	0.655487	1.160385
C 0	-3.611603	0.078537	0.341736
C 0	-3.605682	0.917084	-0.990479
C 0	-2.336380	1.805313	-0.816193

C 0	-1.140700	0.796295	-0.960861
C 0	-1.131775	0.083084	0.472855
C 0	-2.399017	2.161545	0.706726
C 0	-2.455811	0.365204	2.657059
O 0	0.035782	0.406570	1.283661
C 0	-1.200439	2.990555	1.217484
C 0	-3.681534	2.937897	1.094482
C 0	0.289536	1.283691	-1.401077
C 0	1.132553	-0.587280	1.375107
C 0	0.866486	0.335266	-2.471832
C 0	0.423584	2.740067	-1.853043
C 0	1.398500	3.536926	-1.230652
C 0	1.604568	4.863831	-1.612167
C 0	0.835114	5.428879	-2.631180
C 0	-0.137024	4.650742	-3.263580
C 0	-0.337250	3.322754	-2.880096
C 0	0.297195	0.210678	-3.748962
C 0	0.838654	-0.660004	-4.695938
C 0	1.959000	-1.432358	-4.378387
C 0	2.519272	-1.332077	-3.103943
C 0	1.979446	-0.458939	-2.154922
C 0	0.787552	-1.763687	2.054230
O 0	2.228119	-0.234818	0.863937
C 0	1.715195	-2.802612	2.203247
C 0	1.535156	-4.039780	2.882370
C 0	2.598282	-4.997314	2.934998
C 0	2.460541	-6.211929	3.587219
C 0	1.256958	-6.554565	4.229538
C 0	0.196152	-5.634216	4.194200
C 0	0.321564	-4.414917	3.544998
H 0	-3.473450	-0.992600	0.157974
H 0	-4.549759	0.210190	0.891418
H 0	-4.512543	1.522873	-1.082611
H 0	-3.529709	0.281494	-1.878372
H 0	-2.290436	2.667328	-1.480316
H 0	-1.442291	0.039948	-1.691803
H 0	-1.195831	-1.006042	0.366821
H 0	-1.516846	0.691498	3.109833
H 0	-2.560455	-0.713287	2.833389
H 0	-3.301453	0.875015	3.134705
H 0	-0.275162	2.423660	1.151398
H 0	-1.358917	3.246796	2.273682
H 0	-1.120544	3.921936	0.645477
H 0	-3.669006	3.925613	0.615479
H 0	-3.701065	3.092636	2.180237
H 0	-4.604156	2.428177	0.807587
H 0	0.930435	1.175186	-0.522202
H 0	1.996078	3.100098	-0.438004

H 0	2.364441	5.455048	-1.112381
H 0	0.989960	6.460266	-2.928879
H 0	-0.740570	5.076767	-4.058411
H 0	-1.095367	2.738602	-3.386230
H 0	-0.577377	0.794006	-4.011795
H 0	0.384415	-0.737885	-5.678665
H 0	2.379868	-2.111862	-5.112152
H 0	3.374374	-1.944336	-2.837173
H 0	2.376785	-0.414246	-1.143661
H 0	-0.204803	-1.829559	2.481232
H 0	2.686981	-2.628800	1.745697
H 0	3.534760	-4.748413	2.443710
H 0	3.294617	-6.908524	3.601837
H 0	1.150543	-7.505630	4.739548
H 0	-0.741898	-5.880386	4.685242
H 0	-0.514725	-3.724915	3.536911

SCF Energy: -0.12006 hartrees

Optimized Structures of Anion Radical of 14a

A by UB3LYP/6-31G*

Z-Matrix orientation:

C 0	-2.945541	-0.072845	0.903595
C 0	-4.162994	-0.647552	0.116776
C 0	-4.222855	0.215607	-1.182709
C 0	-2.967010	1.110321	-1.038879
C 0	-1.753967	0.138626	-1.241959
C 0	-1.684448	-0.610062	0.149323
C 0	-2.984406	1.441666	0.485291
C 0	-2.953873	-0.406509	2.389450
O 0	-0.482071	-0.338608	0.844193
C 0	-1.803207	2.306229	0.965240
C 0	-4.258514	2.189026	0.938507
C 0	-0.396561	0.716293	-1.745651
C 0	0.085892	-1.426392	1.597488
C 0	0.535385	-0.415405	-2.213242
C 0	-0.521500	1.781982	-2.834579
C 0	0.365402	2.868942	-2.827240
C 0	0.330338	3.846207	-3.822281
C 0	-0.602798	3.760544	-4.856720
C 0	-1.497681	2.689865	-4.878677
C 0	-1.457108	1.715652	-3.879500
C 0	0.328217	-1.085068	-3.428574
C 0	1.177689	-2.111877	-3.840530
C 0	2.257843	-2.492294	-3.041672
C 0	2.472855	-1.837800	-1.829010

C 0	1.622284	-0.808548	-1.421188
C 0	1.248657	-0.998932	2.279770
O 0	-0.461151	-2.535156	1.574326
C 0	2.008682	-1.867371	3.077744
C 0	3.181885	-1.565765	3.821426
C 0	3.837784	-2.582474	4.586441
C 0	4.981644	-2.330719	5.324997
C 0	5.556763	-1.046585	5.355316
C 0	4.935928	-0.027893	4.613937
C 0	3.790131	-0.268494	3.870911
H 0	-4.021927	-1.713974	-0.093475
H 0	-5.086349	-0.562469	0.701782
H 0	-5.140533	0.812256	-1.231445
H 0	-4.192032	-0.391312	-2.095108
H 0	-2.967377	1.980804	-1.700363
H 0	-2.053696	-0.601974	-1.993500
H 0	-1.756348	-1.694550	0.032043
H 0	-2.094284	0.040054	2.898346
H 0	-2.884308	-1.489014	2.540161
H 0	-3.871552	-0.044479	2.872300
H 0	-0.833252	1.844574	0.799179
H 0	-1.883453	2.490448	2.044052
H 0	-1.828415	3.283859	0.464569
H 0	-4.317520	3.170258	0.448471
H 0	-4.223984	2.370087	2.019791
H 0	-5.191100	1.659302	0.729614
H 0	0.106277	1.189407	-0.900986
H 0	1.098785	2.943207	-2.027435
H 0	1.031830	4.676651	-3.786713
H 0	-0.635773	4.521103	-5.633270
H 0	-2.235794	2.612457	-5.673996
H 0	-2.174484	0.900192	-3.907639
H 0	-0.498077	-0.794739	-4.071808
H 0	0.994888	-2.613586	-4.788666
H 0	2.919632	-3.295090	-3.358536
H 0	3.295547	-2.132446	-1.182846
H 0	1.781937	-0.341019	-0.455444
H 0	1.518463	0.048080	2.173996
H 0	1.652084	-2.895477	3.129730
H 0	3.411240	-3.584900	4.579041
H 0	5.440598	-3.142014	5.890259
H 0	6.455109	-0.848816	5.935455
H 0	5.360992	0.976242	4.620209
H 0	3.339752	0.547165	3.311203

SCF Energy: -1390.34584 hartrees

Optimized Structures of Anion Radical of 14a

B by UB3LYP/6-31G*

Z-Matrix orientation:

```
-----  
C 0 -2.130798 0.866714 1.012085  
C 0 -3.331482 0.339066 0.169907  
C 0 -3.270386 1.170578 -1.149429  
C 0 -1.990387 2.019318 -0.945358  
C 0 -0.804916 1.007355 -1.068649  
C 0 -0.850723 0.260437 0.336105  
C 0 -2.074600 2.376007 0.568878  
C 0 -2.251648 0.585785 2.504471  
O 0 0.325089 0.491043 1.084091  
C 0 -0.881516 3.190400 1.107117  
C 0 -3.336304 3.189300 0.932404  
C 0 0.606598 1.538315 -1.473633  
C 0 1.033585 -0.531616 1.809158  
C 0 1.508087 0.387711 -1.956985  
C 0 0.596588 2.670441 -2.500183  
C 0 1.508179 3.726791 -2.355194  
C 0 1.579529 4.762817 -3.287415  
C 0 0.731094 4.769348 -4.395432  
C 0 -0.187469 3.730606 -4.554520  
C 0 -0.252975 2.697464 -3.618195  
C 0 1.343002 -0.198059 -3.221390  
C 0 2.165497 -1.241669 -3.646088  
C 0 3.174362 -1.723358 -2.809647  
C 0 3.344803 -1.151703 -1.549088  
C 0 2.524033 -0.103790 -1.125473  
C 0 0.360336 -1.732971 2.132568  
O 0 2.195007 -0.204636 2.081772  
C 0 1.022430 -2.779587 2.796051  
C 0 0.484818 -4.030777 3.203537  
C 0 1.310120 -4.985504 3.878937  
C 0 0.830170 -6.215836 4.295181  
C 0 -0.508500 -6.585297 4.068283  
C 0 -1.343170 -5.669846 3.407135  
C 0 -0.873016 -4.434738 2.986328  
H 0 -3.242981 -0.739258 -0.007935  
H 0 -4.278046 0.491500 0.701202  
H 0 -4.158707 1.799530 -1.273682  
H 0 -3.203110 0.539261 -2.042755  
H 0 -1.923035 2.879684 -1.615570  
H 0 -1.077530 0.273911 -1.836777  
H 0 -0.971466 -0.816040 0.178329  
H 0 -1.346329 0.888535 3.037918  
H 0 -2.398575 -0.481964 2.700455  
H 0 -3.108170 1.122070 2.933731
```

H 0	0.065002	2.658813	1.048080
H 0	-1.040070	3.435028	2.165237
H 0	-0.799683	4.140335	0.561523
H 0	-3.303909	4.171417	0.441864
H 0	-3.373383	3.370667	2.013290
H 0	-4.278000	2.712082	0.651138
H 0	1.084793	1.930908	-0.575943
H 0	2.175858	3.729400	-1.496704
H 0	2.297700	5.567169	-3.144470
H 0	0.780945	5.575928	-5.123077
H 0	-0.860855	3.724319	-5.408905
H 0	-0.987122	1.908066	-3.754578
H 0	0.572952	0.170898	-3.893387
H 0	2.016953	-1.677185	-4.632187
H 0	3.813690	-2.540924	-3.135406
H 0	4.109940	-1.527298	-0.874542
H 0	2.646271	0.290619	-0.120239
H 0	-0.687698	-1.840591	1.880951
H 0	2.072113	-2.603806	3.025726
H 0	2.350220	-4.721481	4.066208
H 0	1.502258	-6.905365	4.805954
H 0	-0.885712	-7.551453	4.395111
H 0	-2.384491	-5.931870	3.218216
H 0	-1.552277	-3.756104	2.476669

SCF Energy: -1390.33629 hartrees