Aryl to Aryl Palladium Migration in the Heck and Suzuki Coupling of *o*-Halobiaryls

Supporting Information

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Synthetic Procedures

General procedures. All ^1H and ^{13}C NMR spectra were recorded at 300 and 75.5 MHz or 400 and 100 MHz respectively. Thin-layer chromatography was performed using commercially prepared 60-mesh silica gel plates (Whatman K6F), and visualization was effected with short wavelength UV light (254 nm) and a basic KMnO_4 solution [3 g of KMnO_4 + 20 g of K_2CO_3 + 5 mL of NaOH (5%) + 300 mL of H_2O]. All melting points are uncorrected. High resolution mass spectra were recorded on a Kratos MS50TC double focusing magnetic sector mass spectrometer using EI at 70 eV.

Reagents. All reagents were used directly as obtained commercially unless otherwise noted. Anhydrous forms of THF, DME, DMF, diethyl ether, ethyl acetate and hexanes were purchased from Fisher Scientific Co. Tetra-*n*-butylammonium chloride (TBAC) was purchased from Lancaster Synthesis, Inc. 3-Bromoanisole, 1-bromo-2-iodobenzene, diphenylacetylene and ethyl acrylate were purchased from Aldrich Chemical Co., Inc. Cesium pivalate was prepared according to the procedure of Larock and Campo.¹ Compounds **1a**,¹ **2a**,² **3a**,² **1c**,¹ **2c**,² **3c**,² **4a**,² **4c**,² **5**,² **6**,² **7**,² **8**,¹ **9**,¹ and **19**¹ have been reported previously.

Synthesis of the *o*-halobiaryls

***N,N*-Dimethyl-4-(2-iodophenyl)aniline (1b).** Compound **1b** was prepared in two steps from compound **1e**. To a solution of **1e** (0.389 g, 1.19 mmol), $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ (5.0 mg, 0.018 mmol), and activated charcoal (2.4 mg) in methanol (10 mL) under reflux was added $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$ (0.115 g, 3.03 mmol) dropwise over 10 min. The mixture was refluxed for an

additional 14 h and then allowed to cool to room temperature. The reaction mixture was diluted with diethyl ether (50 mL) and the organic layer was washed with water (50 mL). The organic layer was dried (Na_2SO_4), filtered and the solvent evaporated under reduced pressure to obtain a yellow oil [presumed to be 4-(2-iodophenyl)aniline], which without further purification or characterization was dissolved in acetonitrile (8 mL). To this acetonitrile solution was added 37% aq formaldehyde (0.96 mL) and NaBH_3CN (0.230 g, 3.66 mmol). The resulting reaction mixture was stirred at room temperature while glacial acetic acid (0.12 mL) was added dropwise over 10 min. After the addition, the reaction mixture was stirred for 40 min, then another portion of glacial acetic acid (0.12 mL) was added at once and stirring continued for an additional 30 min. The reaction mixture was diluted with diethyl ether (50 mL) and washed with 5% aq NaOH. The organic layer was dried (Na_2SO_4), filtered, and the solvent evaporated under reduced pressure. The residue was purified by chromatography on a silica gel column using 9:1 hexanes/ethyl acetate to afford 36.9 mg (96%) of the indicated compound **1b** as a colorless oil: ^1H NMR (CDCl_3) δ 3.00 (s, 6H), 6.75-6.77 (m, 2H), 6.94-6.98 (m, 1H), 7.23-7.26 (m, 2H), 7.29-7.36 (m, 2H), 7.93 (d, J = 8.0 Hz, 1H); ^{13}C NMR (CDCl_3) δ 40.5, 99.6, 111.5, 128.1, 128.2, 130.1, 130.3, 132.4, 139.5, 146.8, 149.9; IR (CH_2Cl_2) 2917, 2849, 1612, 1525, 1461, 1351 cm^{-1} ; HRMS m/z 323.0176 (calcd for $\text{C}_{14}\text{H}_{14}\text{IN}$, 323.0171).

Ethyl 4-(2-iodophenyl)benzoate (1d). To a solution of 4-(2-iodophenyl)benzaldehyde¹ (0.33 g, 1.07 mmol) in ethanol (10 mL) was added activated MnO_2 (1.90 g, 20 equiv), KCN (0.35 g, 5 equiv) and HOAc (0.20 mL, 3 equiv). The mixture was stirred at room temperature for 1 d and filtered. The organic solution was diluted with EtOAc and washed with brine, dried over anhydrous Na_2SO_4 , filtered and evaporated. The

residue was purified on a silica gel column using 9:1 hexanes/EtOAc to afford 0.353 g (94%) of the desired compound as a colorless oil: ^1H NMR (CDCl_3) δ 1.41 (t, $J = 7.2$ Hz, 3H), 4.40 (q, $J = 7.2$ Hz, 2H), 7.04 (dt, $J = 1.8, 7.8$ Hz, 1H), 7.28 (dd, $J = 1.8, 7.8$ Hz, 1H), 7.37-7.44 (m, 3H), 7.95 (dd, $J = 0.9, 7.8$ Hz, 1H), 8.11 (dt, $J = 8.4, 1.8$ Hz, 2H); ^{13}C NMR (CDCl_3) δ 14.7, 61.3, 98.1, 128.5, 129.5 (2), 129.6, 129.9, 130.1, 139.9, 145.9, 148.7, 166.6; IR (neat, cm^{-1}) 3042, 2970, 1726; HRMS calcd for $\text{C}_{15}\text{H}_{13}\text{IO}_2$: 351.9960. Found: 351.9966.

2-Iodo-4'-nitrobiphenyl (1e). Compound **1e** was prepared by the procedure of Ozasa *et al.*³

***N,N*-Dimethyl-3-iodo-4-phenylaniline (4b).** Compound **4b** was prepared in two steps from 2-iodo-4-nitrobiphenyl (**4e**) by a procedure similar to that used for **1d**. The reaction mixture was purified by chromatography on a silica gel column using 9:1 hexanes/ethyl acetate to afford 38.1 mg (98%) of the indicated compound (**4b**) as a yellow solid: mp 76-77 °C; ^1H NMR (CDCl_3) δ 2.96 (s, 6H), 6.75 (dd, $J = 8.4, 2.8$ Hz, 1H), 7.14 (d, $J = 8.4$ Hz, 1H), 7.26 (d, $J = 2.8$ Hz, 1H), 7.33-7.38 (m, 5H); ^{13}C NMR (CDCl_3) δ 40.5, 99.5, 112.3, 122.9, 127.0, 127.8, 129.8, 130.1, 134.4, 144.3, 150.4; IR (CH_2Cl_2) 2917, 2849, 1598,

Ethyl 3-iodo-4-phenylbenzoate (4d). Compound **4d** was prepared from ethyl 4-iodo-3-nitrobenzoate.⁴ First, a Suzuki coupling of ethyl 4-iodo-3-nitrobenzoate and NaBPh_4 was carried out as follows. NaBPh_4 (1.69 g, 4.94 mmol), ethyl 4-iodo-3-nitrobenzoate (1.38 g, 4.3 mmol), LiCl (0.182 g, 4.3 mmol), $\text{Pd}(\text{OAc})_2$ (0.048 g, 5 mol %), and PPh_3 (0.113 g, 10 mol %) in DMF (10 mL) were stirred under Ar at 70 °C for 2 d. The reaction mixture was diluted with ether and washed with brine. The organic layer was dried (MgSO_4), filtered and evaporated to afford a yellow oil, which is presumed to be crude ethyl 3-nitro-4-phenylbenzoate. The crude ethyl 3-nitro-4-phenylbenzoate was dissolved in a mixture of

DME/EtOH/AcOH (5:4:1, 50 mL) and SnCl₂ (5.71 g, 30.1 mmol) was added. The resulting mixture was stirred at 60 °C under Ar for 16 h, diluted with ether and washed with 10% aq Na₂CO₃. The organic layer was dried (Na₂SO₄), filtered and evaporated. The residue was purified on a silica gel column using 3:1 hexanes/EtOAc to afford 0.93 g (90%) of ethyl 3-amino-4-phenylbenzoate as a yellow oil, which was quickly diazotized and iodinated by the following procedure. To a solution of ethyl 3-amino-4-phenylbenzoate (0.93 g, 3.86 mmol) in DME (10 mL) was added H₂O (8 mL) containing concentrated H₂SO₄ (0.7 mL). The reaction mixture was stirred at 0 °C and NaNO₂ (0.39 g, 5.6 mmol) in H₂O (2 mL) was added dropwise over 30 min. The mixture was stirred for another 20 min at 0 °C and then the mixture was added to NaI (3.0 g, 20.0 mmol) in H₂O (7 mL). The mixture was extracted with ether and washed with 10% aq Na₂S₂O₃. The organic layer was filtered, dried (Na₂SO₄) and evaporated. The residue was purified on a silica gel column using 7:1 hexanes/EtOAc to afford 1.06 g (78%) of compound **4d** as a white solid: mp 76-77 °C; ¹H NMR (CDCl₃) δ 1.41 (t, *J* = 7.2 Hz, 3H), 4.40 (q, *J* = 7.2 Hz, 2H), 7.33-7.37 (m, 3H), 7.41-7.45 (m, 3H), 8.04 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.61 (d, *J* = 1.6 Hz, 1H); ¹³C NMR (CDCl₃) δ 14.4, 61.4, 98.1, 128.2 (2), 129.0, 129.2, 129.9, 130.8, 140.6, 143.4, 150.9, 165.0; IR (neat, cm⁻¹) 2973, 2818, 1722; HRMS calcd for C₁₅H₁₃IO₂: 351.9960. Found: 351.9966. Anal. calcd for C₁₅H₁₃IO₂: C, 51.14; H, 3.34. Found: C, 51.16; H, 3.72.

2-Iodo-4-nitrobiphenyl (4e). Compound **4e** was prepared in two steps from 2-iodo-4-nitroaniline.⁵ First of all, 2-iodo-4-nitroaniline was diazotized by the following procedure. To a solution of 2-iodo-4-nitroaniline (1.09 g, 4.13 mmol), and 48-50% aq HBF₄ (3.0 g) in methanol (20 mL) was added NaNO₂ (0.342 g, 4.96 mmol) in H₂O (0.5 mL) at room temperature. The reaction mixture was stirred for 30 min, and then the reaction mixture was

concentrated to 10 mL by passing a stream of Ar over it. At this point, a yellow solid had precipitated out of solution, and further crystallization was induced by cooling the mixture to -20 °C. The solid was filtered and washed repeatedly with diethyl ether. Recrystallization from methanol/diethyl ether afforded 0.673 g (49%) of 4-nitro-2-iodophenyldiazonium tetrafluoroborate as a yellow solid. 4-Nitro-2-iodophenyldiazonium tetrafluoroborate (82.7 mg, 0.25 mmol) was dissolved in dry DMSO (2.0 mL), then diluted with dry benzene (8.0 mL). The reaction mixture was stirred at 80 °C for 2 h under Ar. The reaction mixture was diluted with diethyl ether (20 mL) and washed with brine (30 mL). The organic layer was dried (Na₂SO₄), filtered and the solvent removed under reduced pressure. The residue was purified by chromatography on a silica gel column using 12:1 hexanes/ethyl acetate to obtain 35.8 mg (44%) of the indicated compound **4e** as a yellow solid: mp 91-92 °C; ¹H NMR (CDCl₃) δ 7.33-7.35 (m, 2H), 7.45-7.48 (m, 4H), 8.25 (dd, *J* = 8.4, 2.4 Hz, 1H), 8.80 (d, *J* = 2.4 Hz, 1H); ¹³C NMR (CDCl₃) δ 97.9, 123.1, 128.4, 128.8, 130.2, 134.5, 142.3, 147.0, 153.1 (one sp² carbon missing due to overlap); IR (CH₂Cl₂) 2918, 2850, 1523, 1349 cm⁻¹; HRMS *m/z* 324.9606 (calcd for C₁₂H₈INO₂, 324.9600); Anal. C, 44.29, H, 2.29; N, 4.11 (calcd for C₁₂H₈INO₂: C, 44.33; H, 2.48; N, 4.34).

3-(2-Iodophenyl)-1-methylindole (12). Compound **12** was prepared in two steps from 2-(2-iodophenyl)acetaldehyde.⁶ A solution of 2-(2-iodophenyl)acetaldehyde (0.216 g, 0.88 mmol), phenylhydrazine (0.105 g, 0.97 mmol) and methanesulfonic acid (17 mg, 0.18 mmol) in ethanol (5 mL) was stirred at room temperature for 40 min under Ar. Then more methanesulfonic acid (0.152 g, 1.58 mmol) was added and the mixture was stirred at 85 °C for 1.5 d under Ar. The reaction mixture was diluted with ether, washed with satd aq NH₄Cl and the organic layer was dried (Na₂SO₄), filtered and evaporated. The residue was purified

on a silica gel column using 3:1 hexanes/EtOAc to afford 0.115 g (41%) of 3-(2-iodophenyl)indole as a yellow oil: ^1H NMR (CDCl_3) δ 6.99 (m, 1H), 7.13-7.17 (m, 1H), 7.21-7.25 (m, 1H), 7.32-7.47 (m, 4H), 7.53 (d, J = 8.0 Hz, 1H), 8.00 (dd, J = 8.0, 0.8 Hz, 1H), 8.18 (br s, 1H); ^{13}C NMR (CDCl_3) δ 100.9, 111.4, 120.2, 122.5, 123.7, 126.6, 128.1, 128.4, 131.5, 135.7, 139.9, 140.0 (two sp^2 carbons missing due to overlap). To a suspension of NaH (0.031 g, 1.3 mmol) in DMF (2.0 mL) at 0 °C was added 3-(2-iodophenyl)indole (0.319 g, 1.0 mmol) in DMF (3.0 mL) and the mixture was stirred at room temperature for 30 min. MeI (1.42 g, 10.0 mmol) in DMF (3 mL) was added and the reaction mixture was stirred at room temperature for 14 h. The reaction mixture was diluted with ether, washed with brine and the organic layer was dried (MgSO_4), filtered and evaporated. The residue was purified on a silica gel column using 5:1 hexanes/EtOAc to afford 0.320 g (96%) of compound **12** as a yellow oil: ^1H NMR (CDCl_3) δ 3.84 (s, 3H), 6.97-7.01 (m, 1H), 7.12-7.16 (m, 1H), 7.22-7.28 (m, 2H), 7.35-7.40 (m, 2H), 7.45 (dd, J = 7.6, 1.6 Hz, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.99 (dd, J = 7.6, 0.8 Hz, 1H); ^{13}C NMR (CDCl_3) δ 33.1, 100.8, 109.5, 118.5, 119.7, 120.3, 122.0, 127.0, 128.1, 128.2, 128.4, 131.5, 136.6, 139.9, 140.1; IR (neat, cm^{-1}) 3050, 2922, 1547; HRMS calcd for $\text{C}_{15}\text{H}_{12}\text{IN}$: 333.0014. Found: 333.0024.

2-Iodo-3',5'-dimethylbiphenyl (13). 2-Iodo-3',5'-dimethylbiphenyl (**13**) was prepared by a procedure reported by Hart.⁷ A solution of 2-bromiodobenzene (1.415 g, 5.0 mmol) in THF (10 mL) was added slowly (90 min) to a solution of 3,5-dimethylphenylmagnesium bromide [prepared from 1-bromo-3,5-dimethylbenzene (1.85 g, 10 mmol) and Mg (0.246 g, 10 mmol) in THF (30 mL)], and the mixture was stirred under Ar for an additional 14 h at room temperature. The reaction was quenched by adding I_2 (3.8 g, 15 mmol), and the mixture was stirred for an additional 30 min at room temperature. The

excess I₂ was destroyed by adding 10% aq NaHSO₃ (35 mL) and the organic layer was separated and rewashed with brine (20 mL). Finally, the organic layer was dried (MgSO₄), filtered, and the solvent removed under reduced pressure. The residue was chromatographed using hexanes to afford 0.836 g (54%) of the desired compound **13** as a clear oil: ¹H NMR (CDCl₃) δ 2.36 (s, 6H), 6.95-7.02 (m, 4H), 7.33-7.82 (m, 1H), 7.92-7.94 (m, 1H); ¹³C NMR (CDCl₃) δ 21.6, 98.9, 127.3, 128.3, 128.8, 129.4, 130.3, 137.6, 139.6, 144.3, 147.1; IR (CH₂Cl₂) 2917, 2849, 1602, 1461, 1015 cm⁻¹; HRMS *m/z* 308.0070 (calcd for C₁₄H₁₃I, 308.0062).

2-Iodo-2'-methylbiphenyl (16). Compound **16** was prepared by a procedure reported by Hart.⁷ A solution of 2-bromoiodobenzene (1.415 g, 5.0 mmol) in THF (10 mL) was added slowly (90 min) to a solution of 2-methylphenylmagnesium bromide [prepared from 2-bromotoluene (1.71 g, 10 mmol) and Mg (0.246 g, 10 mmol) in THF (30 mL)], and the mixture was stirred under Ar for an additional 14 h at room temperature. The reaction was quenched by adding I₂ (3.8 g, 15 mmol), and the mixture was stirred for an additional 30 min at room temperature. The excess I₂ was destroyed by adding 10% aq NaHSO₃ (35 mL) and the organic layer was separated and rewashed with brine (20 mL). Finally, the organic layer was dried (MgSO₄), filtered, and the solvent removed under reduced pressure. The residue was chromatographed using hexanes to afford 0.97 g (66%) of the desired compound **16** as a clear oil: ¹H NMR (CDCl₃) δ 2.07 (s, 3H), 7.01-7.07 (m, 2H), 7.20-7.31 (m, 4H), 7.36-7.40 (m, 1H), 7.92-7.94 (m, 1H); ¹³C NMR (CDCl₃) δ 20.1, 100.1, 125.6, 128.0, 128.1, 128.7, 129.2, 129.7, 129.9, 135.7, 138.9, 144.4, 146.8; IR (CH₂Cl₂) 3056, 3018, 2921, 1461, 1428 cm⁻¹; HRMS *m/z* 293.9910 (calcd for C₁₄H₁₃I, 293.9906).

2-Iodo-3'-methoxybiphenyl (26). Compound **26** was prepared by a procedure reported by Hart.⁷ A solution of 2-bromiodobenzene (1.415 g, 5.0 mmol) in THF (10 mL) was added slowly (90 min) to a solution of 3-methoxyphenylmagnesium bromide [prepared from 3-bromoanisole (1.87 g, 10 mmol) and Mg (0.246 g, 10 mmol) in THF (30 mL)], and the mixture was stirred under Ar for an additional 14 h at room temperature. The reaction was quenched by adding I₂ (3.8 g, 15 mmol), and the mixture was stirred for an additional 30 min at room temperature. The excess I₂ was destroyed by adding 10% aq NaHSO₃ (35 mL) and the organic layer was separated and rewashed with brine (20 mL). Finally, the organic layer was dried (MgSO₄), filtered, and the solvent removed under reduced pressure. The residue was chromatographed using 30:1 hexanes/ethyl acetate to afford 0.620 g (40%) of the desired compound **26** as a clear oil: ¹H NMR (CDCl₃) δ 3.84 (s, 3H), 6.88-6.95 (m, 3H), 7.01-7.05 (m, 1H), 7.29-7.38 (m, 3H), 7.95 (dd, *J* = 8.0, 1.2 Hz, 1H); ¹³C NMR (CDCl₃) δ 55.4, 98.5, 113.4, 115.0, 121.8, 128.1, 128.9, 129.1, 130.1, 139.6, 145.5, 146.5, 159.1; HRMS *m/z* 309.9859 (calcd for C₁₃H₁₁IO, 309.9855).

Heck reactions

The following procedures are representative of the palladium-catalyzed Heck reactions with ethyl acrylate.

Migration reaction conditions (procedure C): The appropriate aryl halide (0.25 mmol), Pd(OAc)₂ (2.8 mg, 0.0125 mmol), 1,1-bis(diphenylphosphino)methane (dppm) (4.8 mg, 0.0125 mmol), CsO₂CCMe₃ (CsPiv) (0.117 g, 0.5 mmol) and ethyl acrylate (0.025 g, 0.25 mmol) in DMF (4.0 ml) under Ar at 100 °C were stirred for the specified length of time. The reaction mixture was then cooled to room temperature, diluted with diethyl ether (35

mL) and washed with brine (30 mL). The aqueous layer was reextracted with diethyl ether (15 mL). The organic layers were combined, dried (MgSO_4), filtered, and the solvent removed under reduced pressure. The residue was purified by column chromatography on a silica gel column.

Migration reaction conditions (procedure D): The appropriate aryl halide (0.25 mmol), $\text{Pd}(\text{OAc})_2$ (2.8 mg, 0.0125 mmol), 1,1-bis(diphenylphosphino)methane (dppm) (4.8 mg, 0.0125 mmol), $\text{CsO}_2\text{CCMe}_3$ (CsPiv) (0.117 g, 0.5 mmol) and ethyl acrylate (0.025 g, 0.25 mmol) in wet DMF (5% H_2O by volume) (4.0 mL) under Ar at 100 °C were stirred for the specified length of time. The reaction mixture was then cooled to room temperature, diluted with diethyl ether (35 mL) and washed with brine (30 mL). The aqueous layer was reextracted with diethyl ether (15 mL). The organic layers were combined, dried (MgSO_4), filtered, and the solvent removed under reduced pressure. The residue was purified by column chromatography on a silica gel column.

Non-migration reaction conditions (procedure A):⁶ The appropriate aryl iodide (0.25 mmol), $\text{Pd}(\text{OAc})_2$ (2.8 mg, 0.0125 mmol), *n*- Bu_4NCl (0.0694 g, 0.25 mmol), NaHCO_3 (0.042 g, 0.5 mmol) and ethyl acrylate (0.10 g, 1.0 mmol) in DMF (1 mL) under Ar at 100 °C were stirred for the specified length of time. The reaction mixture was then cooled to room temperature, diluted with diethyl ether (35 mL) and washed with brine (30 mL). The aqueous layer was reextracted with diethyl ether (15 mL). The organic layers were combined, dried (MgSO_4), filtered, and the solvent removed under reduced pressure. The residue was purified by column chromatography on a silica gel column.

Non-migration reaction conditions (procedure B): The appropriate aryl iodide (0.25 mmol), $\text{Pd}(\text{OAc})_2$ (2.8 mg, 0.0125 mmol), *n*- Bu_4NCl (0.0694 g, 0.25 mmol), Et_3N (50.5

mg, 0.5 mmol) and ethyl acrylate (0.10 g, 1.0 mmol) in DMF (1 mL) under Ar at 100 °C were stirred for the specified length of time. The reaction mixture was then cooled to room temperature, diluted with diethyl ether (35 mL) and washed with brine (30 mL). The aqueous layer was reextracted with diethyl ether (15 mL). The organic layers were combined, dried (MgSO₄), filtered, and the solvent removed under reduced pressure. The residue was purified by column chromatography on a silica gel column.

Ethyl *E*-3-(4'-dimethylaminobiphen-2-yl)acrylate (2b). *N,N*-Dimethyl-4-(2-iodophenyl)aniline (**1b**) (80.8 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 1 d. The reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 59.0 mg (80%) of the indicated compound as a yellow solid: mp 117-118 °C; ¹H NMR (CDCl₃) δ 1.30 (t, *J* = 7.0 Hz, 3H), 3.01 (s, 6H), 4.22 (q, *J* = 7.2 Hz, 2H), 6.39 (d, *J* = 15.6 Hz, 1H), 6.78-6.80 (m, 2H), 7.20-7.22 (m, 2H), 7.31-7.40 (m, 3H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.84 (d, *J* = 16.0 Hz, 1H); ¹³C NMR (CDCl₃) δ 14.4, 40.6, 60.3, 112.2, 118.5, 126.7, 126.9, 127.7, 129.8, 130.4, 130.7, 132.6, 143.2, 144.7, 150.0, 167.2; IR (CH₂Cl₂) 2975, 2926, 2857, 1715, 1612, 1631, 1526 cm⁻¹; HRMS *m/z* 295.1580 (calcd for C₁₉H₂₁NO₂, 295.1572); Anal. C, 77.05, H, 7.29; N, 4.57 (calcd for C₁₉H₂₁NO₂: C, 77.26; H, 7.17; N, 4.77).

Ethyl *E*-3-(4-dimethylaminobiphen-2-yl)acrylate (3b). *N,N*-Dimethyl-3-iodo-4-phenylaniline (**4b**) (80.8 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 1 d. The reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 73.8 mg (100%) of the indicated compound as a yellow oil: ¹H NMR (CDCl₃) δ 1.28 (t, *J* = 7.2 Hz, 3H), 3.01 (s, 6H), 4.21 (q, *J* = 7.2 Hz, 2H), 6.39 (d, *J* = 15.6 Hz, 1H), 6.85 (dd, *J* = 8.8, 2.8 Hz, 1H), 6.97 (d, *J* = 2.8 Hz,

1H), 7.24-7.34 (m, 4H), 7.38-7.42 (m, 2H), 7.77 (d, $J = 16.0$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.4, 40.6, 60.4, 109.8, 114.7, 118.7, 126.8, 128.2, 130.0, 131.3, 131.6, 133.1, 140.2, 145.1, 149.8, 167.1; IR (CH_2Cl_2) 2975, 2920, 1711, 1632, 1605, 1174 cm^{-1} ; HRMS m/z 295.1577 (calcd for $\text{C}_{19}\text{H}_{21}\text{NO}_2$, 295.1572).

Ethyl *E*-3-(4'-dimethylaminobiphen-2-yl)acrylate (2b) and ethyl *E*-3-(4-dimethylaminobiphen-2-yl)acrylate (3b). Compound **1b** (80.8 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 1 d. The reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 66.4 mg (90%) of the indicated compounds as a clear oil in a 55:45 ratio. Similarly, compound **4b** (80.8 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our standard migration reaction conditions A for 1 d. The reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 68.6 mg (93%) of the indicated compounds as a clear oil in a 49:51 ratio.

Ethyl *E*-3-(4'-ethoxycarbonylbiphen-2-yl)acrylate (2d). Ethyl 4-(2-iodophenyl)benzoate (**1d**) (76.2 mg, 0.25 mmol) was allowed to react for 2 d under non-migration reaction conditions (procedure A) with ethyl acrylate. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 58.3 mg (72%) of the indicated compound (**2d**) as a clear oil: ^1H NMR (CDCl_3) δ 1.28 (t, $J = 7.0$ Hz, 3H), 1.42 (t, $J = 7.2$ Hz, 3H), 4.21 (q, $J = 7.2$ Hz, 2H), 4.42 (q, $J = 7.2$ Hz, 2H), 6.41 (d, $J = 15.6$ Hz, 1H), 7.36-7.46 (m, 5H), 7.66 (d, $J = 16.0$ Hz, 1H), 7.70-7.72 (m, 1H), 8.11-8.13 (m, 2H); ^{13}C NMR (CDCl_3) δ 14.3, 14.4, 60.5, 61.1, 119.8, 127.0, 128.3, 129.6, 129.7, 129.9, 130.0, 130.4, 132.7, 141.8, 143.2, 144.5, 166.4, 166.7; IR (CH_2Cl_2) 2880, 2933, 1713, 1633 cm^{-1} ; HRMS m/z 324.1368 (calcd for $\text{C}_{20}\text{H}_{20}\text{O}_4$, 324.1362).

Ethyl *E*-3-(4-ethoxycarbonylbiphen-2-yl)acrylate (3d). Ethyl 3-iodo-4-phenylbenzoate (**4d**) (76.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 80.2 mg (99%) of the indicated compound (**3d**) as a clear oil: ^1H NMR (CDCl_3) δ 1.30 (t, $J = 7.2$ Hz, 3H), 1.43 (t, $J = 7.0$ Hz, 3H), 4.22 (q, $J = 7.2$ Hz, 2H), 4.42 (q, $J = 7.2$ Hz, 2H), 6.52 (d, $J = 16.0$ Hz, 1H), 7.32-7.33 (m, 2H), 7.42-7.48 (m, 4H), 7.72 (d, $J = 16.0$ Hz, 1H), 8.08-8.10 (m, 1H), 8.38 (s, 1H); ^{13}C NMR (CDCl_3) δ 14.3, 14.4, 60.6, 61.3, 120.4, 128.2, 128.5, 129.7, 129.9, 130.5, 130.7, 132.9, 139.0, 142.8, 146.9, 166.0, 166.7 (one sp^2 carbon missing due to overlap) ; IR (CH_2Cl_2) 2980, 1717, 1636, 1285, 1245 cm^{-1} ; HRMS m/z 324.1368 (calcd for $\text{C}_{20}\text{H}_{20}\text{O}_4$, 324.1362).

Ethyl *E*-3-(4'-ethoxycarbonylbiphen-2-yl)acrylate (2d) and ethyl *E*-3-(4-ethoxycarbonylbiphen-2-yl)acrylate (3d). Compound **1d** (76.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 69.6 mg (86%) of the indicated compounds as a clear oil in a 48:52 ratio. Similarly, compound **4d** (76.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 67.2 mg (83%) of the indicated compounds as a clear oil in a 42:58 ratio.

Ethyl *E*-3-(4'-nitrobiphen-2-yl)acrylate (2e). Compound **1e** (81.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure B). After 1 d, the reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to

afford 63.1 mg (85%) of the indicated compound **2e** as a yellow oil: ^1H NMR (CDCl_3) δ 1.29 (t, $J = 7.0$ Hz, 3H), 4.22 (q, $J = 7.2$ Hz, 2H), 6.43 (d, $J = 16.0$ Hz, 1H), 7.36-7.38 (m, 1H), 7.46-7.51 (m, 4H), 7.60 (d, $J = 15.6$ Hz, 1H), 7.72-7.74 (m, 1H), 8.29-8.32 (m, 2H); ^{13}C NMR (CDCl_3) δ 14.3, 60.7, 120.5, 123.6, 127.3, 129.0, 130.1, 130.3, 130.7, 132.7, 140.3, 142.4, 146.7, 147.3, 166.6; IR (CH_2Cl_2) 2917, 1710, 1517, 1348, 1314, 1179 cm^{-1} ; HRMS m/z 297.1010 (calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_4$, 297.1001).

Ethyl *E*-3-(4-nitrobiphen-2-yl)acrylate (3e). Compound **4e** (81.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure B). After 1 d, the reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 66.1 mg (89%) of the indicated compound **3e** as a yellow solid: mp = 118-119 $^\circ\text{C}$, ^1H NMR (CDCl_3) δ 1.31 (t, $J = 7.2$ Hz, 3H), 4.24 (q, $J = 7.2$ Hz, 2H), 6.55 (d, $J = 15.9$ Hz, 1H), 7.31-7.34 (m, 2H), 7.46-7.56 (m, 4H), 7.69 (d, $J = 15.9$ Hz, 1H), 8.26 (dd, $J = 8.4, 2.4$ Hz, 1H), 8.55 (d, $J = 2.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.5, 61.0, 122.2, 122.2, 124.2, 128.9, 129.1, 129.7, 131.8, 134.4, 138.1, 141.6, 147.5, 148.8, 166.3; IR (CH_2Cl_2) 2974, 2917, 2849, 1719, 1523, 1347, 1179, 1118 cm^{-1} ; HRMS m/z 297.1010 (calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_4$, 297.1001); Anal. C, 68.41; H, 4.84; N, 4.51 (calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_4$: C, 68.68; H, 5.09; N, 4.71).

Ethyl *E*-3-(4'-nitrobiphen-2-yl)acrylate (2e) and ethyl *E*-3-(4-nitrobiphen-2-yl)acrylate (3e). Compound **1e** (81.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure D) for 2.5 d. The reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 34.2 mg (46%) of the indicated compounds as a yellow oil in a 39:61 ratio. In addition, we obtained 19.9 mg (40%) of 4-nitrobiphenyl as a yellow solid with spectral properties identical to those previously reported.¹¹ Similarly, compound **4e** (81.2 mg, 0.25 mmol) was allowed to react

with ethyl acrylate under our migration reaction conditions (procedure D) for 2.5 d. The reaction mixture was chromatographed using 5:1 hexanes/ethyl acetate to afford 27.5 mg (37%) of the indicated compounds as a yellow oil in a 33:67 ratio. In addition, we obtained 24.9 mg (50%) of 4-nitrobiphenyl as a yellow solid with spectral properties identical to those previously reported.¹¹

Ethyl *E*-3-(3-phenylbenzofuran-2-yl)acrylate (6). Compound **5** (80.0 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 62.1 mg (85%) of the indicated compound as a white solid: mp 84-85 °C, ¹H NMR (CDCl₃) δ 1.32 (t, *J* = 7.2 Hz, 3H), 4.25 (q, *J* = 7.2 Hz, 2H), 6.68 (d, *J* = 15.6 Hz, 1H), 7.25-7.29 (m, 1H), 7.40-7.54 (m, 7H), 7.63-7.68 (m, 2H); ¹³C NMR (CDCl₃) δ 14.4, 60.7, 111.6, 119.4, 121.0, 123.5, 125.7, 127.0, 128.4, 128.4, 129.2, 129.6, 130.3, 131.2, 148.3, 155.0, 167.0; IR (CH₂Cl₂) 3062, 2979, 1709, 1628, 1450 cm⁻¹; HRMS *m/z* 292.1104 (calcd for C₁₉H₁₆O₃, 292.1099). Similarly, compound **8** (80.0 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C). The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 57.0 mg (78%) of the indicated compound as a yellow solid: mp 82-84 °C.

Ethyl *E*-3-[2-(benzofuran-3-yl)phenyl]acrylate (7). Compound **8** (80.0 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) at 80 °C for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 54.8 mg (75%) of the indicated compound as a clear oil: ¹H NMR (CDCl₃) δ 1.24 (t, *J* = 7.0 Hz, 3H), 4.18 (q, *J* = 7.2 Hz, 2H), 6.44 (d, *J* = 16.0 Hz, 1H), 7.24-7.28 (m, 1H), 7.33-7.58 (m, 6H), 7.60 (s, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.86 (d, *J* = 15.6

Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.3, 60.5, 111.8, 119.8, 119.8, 120.5, 123.2, 124.9, 127.1, 127.6, 128.2, 130.1, 130.7, 132.2, 133.7, 143.1, 143.5, 155.3, 166.8; IR (CH_2Cl_2) 3060, 2979, 1711, 1633, 1452 cm^{-1} ; HRMS m/z 292.1104 (calcd for $\text{C}_{19}\text{H}_{16}\text{O}_3$, 292.1099).

Ethyl *E*-3-(1-methyl-3-phenylindol-2-yl)acrylate (10). Compound **9** (83.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 1 d. The reaction mixture was chromatographed using 3:1 hexanes/ethyl acetate to afford 71.2 mg (94%) of the indicated compound **10** as a yellow oil: ^1H NMR (CDCl_3) δ 1.29 (t, $J = 7.2$ Hz, 3H), 3.90 (s, 3H), 4.22 (q, $J = 7.2$ Hz, 2H), 6.23 (d, $J = 16.4$ Hz, 1H), 7.12-7.14 (m, 1H), 7.33-7.39 (m, 3H), 7.45-7.48 (m, 4H), 7.62 (d, $J = 8.0$ Hz, 1H), 7.84 (d, $J = 16.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.4, 31.7, 60.6, 109.7, 118.7, 120.6, 120.6, 122.7, 124.6, 127.0, 127.2, 128.8, 130.4, 131.1, 133.3, 134.2, 139.1, 167.2; IR (CH_2Cl_2) 3057, 2975, 2927, 1708, 1625, 1369, 1289, 1180 cm^{-1} ; HRMS m/z 305.1420 (calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_2$, 305.1416).

Ethyl *E*-3-(2-(1-methylindol-3-yl)phenyl)acrylate (11). Compound **12** (83.2 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) at 75 $^\circ\text{C}$ for 2 d. The reaction mixture was chromatographed using 3:1 hexanes/ethyl acetate to afford 64.4 mg (85%) of the indicated compound as a white solid: mp 130-131 $^\circ\text{C}$; ^1H NMR (CDCl_3) δ 1.26 (t, $J = 7.2$ Hz, 3H), 3.85 (s, 3H), 4.19 (q, $J = 7.2$ Hz, 2H), 6.43 (d, $J = 16.0$ Hz, 1H), 7.01 (s, 1H), 7.14-7.18 (m, 1H), 7.27-7.39 (m, 3H), 7.42-7.46 (m, 1H), 7.60-7.64 (m, 2H), 7.73 (d, $J = 8.0$ Hz, 1H), 7.97 (d, $J = 16.0$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.4, 33.0, 60.3, 109.5, 113.9, 118.5, 120.0, 120.1, 122.2, 126.6, 127.0, 127.4, 129.4, 129.9, 131.0, 133.2, 136.0, 137.0, 144.6, 167.2; IR (CH_2Cl_2) 2918, 2848, 1712,

1631, 1314 cm^{-1} ; HRMS m/z 305.1420 (calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_2$, 305.1416); Anal. C, 78.36; H, 6.28; N, 4.45 (calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_2$: C, 78.66; H, 6.27; N, 4.59).

Ethyl *E*-3-(3',5'-dimethylbiphen-2-yl)acrylate (14). Compound **13** (77.0 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 69.0 mg (97%) of the indicated compound **14** as a clear oil: ^1H NMR (CDCl_3) δ 1.28 (t, $J = 7.2$ Hz, 3H), 2.36 (s, 6H), 4.20 (q, $J = 7.2$ Hz, 2H), 6.38 (d, $J = 16.0$ Hz, 1H), 6.92 (s, 2H), 7.02 (s, 1H), 7.33-7.41 (m, 3H), 7.67-7.69 (m, 1H), 7.75 (d, $J = 15.6$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.4, 21.4, 60.3, 118.9, 126.6, 127.5, 127.8, 129.2, 129.8, 130.5, 132.6, 137.8, 139.9, 143.3, 143.9, 167.0; IR (CH_2Cl_2) 2918, 2976, 1712, 1632, 1313 cm^{-1} ; HRMS m/z 280.1468 (calcd for $\text{C}_{19}\text{H}_{20}\text{O}_2$, 280.1463).

Ethyl *E*-3-(2'-methylbiphen-2-yl)acrylate (17). Compound **16** (73.5 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 61.2 mg (92%) of the indicated compound **17** as a yellow oil: ^1H NMR (CDCl_3) δ 1.24 (t, $J = 7.2$ Hz, 3H), 2.03 (s, 3H), 4.16 (q, $J = 7.2$ Hz, 2H), 6.33 (d, $J = 16.0$ Hz, 1H), 7.10 (d, $J = 7.2$ Hz, 1H), 7.20-7.29 (m, 4H), 7.37-7.44 (m, 3H), 7.70-7.72 (m, 1H); ^{13}C NMR (CDCl_3) δ 14.3, 20.1, 60.4, 119.0, 125.7, 126.2, 127.7, 128.0, 129.8, 129.9, 130.1, 130.5, 133.0, 136.1, 139.6, 142.9, 143.0, 166.9; IR (CH_2Cl_2) 3061, 2978, 2920, 1713, 1633, 1177 cm^{-1} ; HRMS m/z 266.1312 (calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2$, 266.1307).

Ethyl *E*-3-(2'-methylbiphen-2-yl)acrylate (17) and ethyl *E*-3-(6-methylbiphen-2-yl)acrylate (18). Compound **16** (73.5 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 1 d. The reaction mixture

was chromatographed using 7:1 hexanes/ethyl acetate to afford 60.5 mg (91%) of the indicated compounds as a yellow oil in a 65:35 ratio. Minor isomer **18**: ^1H NMR (CDCl_3) δ 2.08 (s, 3H), 6.27 (d, $J = 16.0$ Hz, 1H), 7.54-7.56 (m, 1H) as characteristic peaks; ^{13}C NMR (CDCl_3) δ 20.9, 60.3, 118.8, 123.8, 127.4, 127.5, 128.5, 129.7, 131.5, 133.4, 137.0, 138.9, 142.8, 143.9, 143.9 as characteristic peaks; HRMS m/z 266.1312 (calcd for $\text{C}_{18}\text{H}_{18}\text{O}_2$, 266.1307).

Ethyl *E*-3-(3-methoxybiphen-2-yl)acrylate (20). Compound **19** (77.5 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 2 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 55.1 mg (78%) of the indicated compound **20** as a clear oil: ^1H NMR (CDCl_3) δ 1.25 (t, $J = 7.2$ Hz, 3H), 3.94 (s, 3H), 4.16 (q, $J = 7.2$ Hz, 2H), 6.61 (d, $J = 16.4$ Hz, 1H), 6.94-6.96 (m, 2H), 7.28-7.41 (m, 6H), 7.63 (d, $J = 16.4$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.3, 55.7, 60.2, 110.0, 121.5, 122.4, 123.0, 127.5, 128.2, 129.9, 130.0, 139.8, 140.6, 145.5, 159.3, 168.0; IR (CH_2Cl_2) 3054, 2985, 2926, 1705, 1265, cm^{-1} ; HRMS 282.1256 m/z (calcd for $\text{C}_{18}\text{H}_{18}\text{O}_3$, 282.1256).

Ethyl *E*-3-(3'-methoxybiphen-2-yl)acrylate (21). Compound **26** (77.5 mg, 0.25 mmol) was allowed to react with ethyl acrylate under non-migration reaction conditions (procedure A) for 2 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 60.0 mg (85%) of the indicated compound as a clear oil: ^1H NMR (CDCl_3) δ 1.28 (t, $J = 7.2$ Hz, 3H), 3.83 (s, 3H), 4.21 (q, $J = 7.2$ Hz, 2H), 6.39 (d, $J = 16.0$ Hz, 1H), 6.85-6.95 (m, 3H), 7.32-7.43 (m, 4H), 7.68-7.70 (m, 1H), 7.75 (d, $J = 16.0$ Hz, 1H); ^{13}C NMR (CDCl_3) δ 14.3, 55.4, 60.4, 113.4, 115.4, 119.2, 122.4, 126.8, 127.8, 129.3, 129.8,

130.4, 132.7, 141.3, 142.8, 143.8, 159.4, 166.9; IR (CH₂Cl₂) 3061, 2980, 1711, 1632, 1314, 1177, cm⁻¹; HRMS *m/z* (calcd for C₁₈H₁₈O₃, 282.1256).

Ethyl *E*-3-(5-methoxybiphen-2-yl)acrylate (22). An authentic sample of compound **22** was prepared in two steps from 2-iodo-4-methoxybenzaldehyde⁸ [mp 113-114 °C; ¹H NMR (CDCl₃) δ 3.88 (s, 3H), 6.99 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.85 (d, *J* = 8.8 Hz, 1H), 9.93 (s, 1H); ¹³C NMR (CDCl₃) δ 55.9, 102.4, 114.9, 125.4, 128.6, 131.6, 164.4, 194.5] in the following manner. 2-Iodo-4-methoxybenzaldehyde (0.262 g, 1.0 mmol), Pd(OAc)₂ (11.2 mg, 0.05 mmol), PPh₃ (26.2 mg, 0.1 mmol), CsF (0.334 g, 2.2 mmol) and phenylboronic acid (0.146 g, 1.2 mmol) in DME (5 ml) under Ar at 90 °C were stirred for 3 h. The reaction mixture was then cooled to room temperature, diluted with diethyl ether (35 mL) and washed with brine (30 mL). The aqueous layer was reextracted with diethyl ether (15 mL). The organic layers were combined, dried (MgSO₄), filtered, and the solvent removed under reduced pressure. The residue was purified by column chromatography on a silica gel column using 7:1 hexanes/ethyl acetate to afford 21.0 mg (99%) of 2-phenyl-4-methoxybenzaldehyde as a clear oil: ¹H NMR (CDCl₃) δ 3.91 (s, 3H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.99-7.02 (m, 1H), 7.38-7.47 (m, 5H), 8.03 (d, *J* = 8.8 Hz, 1H), 9.84 (d, *J* = 0.4 Hz, 1H); ¹³C NMR (CDCl₃) δ 55.7, 114.0, 115.2, 127.4, 128.3, 128.4, 129.9, 130.0, 137.9, 148.6, 163.6, 191.1. 2-Phenyl-4-methoxybenzaldehyde (53.0 mg, 0.25 mmol) and (carboethoxymethylene)triphenylphosphorane (0.1305 g, 0.375 mmol) in CH₂Cl₂ (5 ml) were stirred at 60 °C under argon for 15 h. The reaction mixture was allowed to cool to room temperature and the solvent evaporated under reduced pressure. The resulting yellow oil was purified by column chromatography on a silica gel column using 1:9 ethyl acetate/hexanes to afford 43.7 mg (62%) of the desired compound **22** as a clear oil: ¹H NMR (CDCl₃) δ 1.27 (t,

$J = 7.2$ Hz, 3H), 3.85 (s, 3H), 4.18 (q, $J = 7.2$ Hz, 2H), 6.29 (d, $J = 15.9$ Hz, 1H), 6.87 (d, $J = 2.7$ Hz, 1H), 6.92-6.95 (m, 1H), 7.29-7.33 (m, 2H), 7.39-7.44 (m, 3H), 7.64-7.69 (m, 2H); ^{13}C NMR (CDCl_3) δ 14.5, 55.7, 60.4, 114.2, 115.4, 117.0, 125.6, 127.9, 128.5, 128.5, 129.9, 140.1, 143.4, 145.1, 160.9, 167.4; IR (CH_2Cl_2) 3056, 2978, 2937, 1709, 1630, 1600, 1484 cm^{-1} ; HRMS m/z (calcd for $\text{C}_{18}\text{H}_{18}\text{O}_3$, 282.1256).

Ethyl *E*-3-(3-methoxybiphen-2-yl)acrylate (20), ethyl *E*-3-(3'-methoxybiphen-2-yl)acrylate (21), and ethyl *E*-3-(5-methoxybiphen-2-yl)acrylate (22). Compound **19** (77.5 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our migration reaction conditions (procedure C) for 2 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 68.5 mg (97%) of the indicated compounds as a clear oil in a 53:38:9 ratio. Similarly, compound **26** (77.5 mg, 0.25 mmol) was allowed to react with ethyl acrylate under our standard migration reaction conditions (Procedure C) for 1 d. The reaction mixture was chromatographed using 7:1 hexanes/ethyl acetate to afford 61.3 mg (87%) of the indicated compounds as a clear oil in a 25:62:13 ratio.

Suzuki reactions

General Procedure for the Suzuki Coupling of *o*-Iodobiphenyls with Arylboronic Acids under the Conditions Described by Wright et al⁹ (Suzuki Non-migration Conditions): To a 2-dram vial was added the *o*-iodobiphenyl (0.25 mmol), the arylboronic acid (0.30 mmol, 1.2 equiv), $\text{Pd}(\text{OAc})_2$ (2.8 mg, 5 mol %), PPh_3 (6.5 mg, 10 mol %), CsF (84.0 mg, 2.2 equiv) and DME (1.0 mL). The mixture was flushed with Ar and stirred at 90 °C in an oil bath. The completion of the reaction was determined by the observation of palladium

black. The reaction mixture was cooled and purified directly by column chromatography on a silica gel column.

General Procedure for the Suzuki Coupling of *o*-Iodobiphenyls with Arylboronic Acids under Migration Conditions (Suzuki Migration Conditions): To a 2-dram vial was added the *o*-iodobiphenyl (0.25 mmol), the arylboronic acid (0.35 mmol, 1.4 equiv), Pd(OAc)₂ (2.8 mg, 5 mol %), (Ph₂P)₂CH₂ (dppm, 4.8 mg, 5 mol %), CsO₂CCMe₃ (CsPiv, 117 mg, 2.0 equiv), Me₃CCO₂H (PA, 51 mg, 2 equiv), H₂O (90 mg, 20 equiv) and DMF (4.0 mL). The mixture was flushed with Ar and stirred at 100 °C in an oil bath. The completion of the reaction was determined by the observation of palladium black. The reaction mixture was cooled, diluted with ether and washed with satd aq NaHCO₃. The organic layer was dried (Na₂SO₄), filtered and evaporated. The residue was purified by column chromatography on a silica gel column and the molar ratio of the products was determined by ¹H NMR spectroscopic analysis.

Methyl 4''-methyl-*o*-terphenyl-4-carboxylate (28a). This compound was prepared employing **1a** and **27a** under Suzuki non-migration conditions for 8 h. The reaction mixture was chromatographed using 9:1 hexanes/EtOAc to afford a 62% yield of the indicated compound as a colorless oil: ¹H NMR (CDCl₃) δ 2.30 (s, 3H), 3.89 (s, 3H), 6.97-7.04 (m, 4H), 7.20-7.23 (m, 2H), 7.40-7.44 (m, 4H), 7.87-7.90 (m, 2H); ¹³C NMR (CDCl₃) δ 21.3, 52.3, 127.6, 128.3 (2), 129.0, 129.4, 129.9, 130.1, 130.6, 131.0, 136.6, 138.3, 139.7, 140.9, 146.9, 167.4; IR (neat, cm⁻¹) 3023, 2918, 1724; HRMS calcd for C₂₁H₁₈O₂: 302.1307. Found: 302.1313.

4''-Methyl-*o*-terphenyl. This compound was prepared employing **1a** and **27b** under Suzuki non-migration conditions for 40 h. The reaction mixture was chromatographed using

50:1 hexanes/EtOAc to afford an 85% yield of the indicated compound as a colorless oil, which crystallizes upon cooling and standing: mp 74-75 °C (lit.¹⁰ mp 74-75 °C); ¹³C NMR (CDCl₃) δ 21.4, 126.7, 127.5, 127.7, 128.1, 128.9, 130.0, 130.2, 130.9, 136.3, 138.8, 140.78, 140.79, 142.0 (one sp² carbon missing due to overlap); all other spectral properties are identical to those previously reported.^{10,11}

4-Methoxy-4''-methyl-*o*-terphenyl. This compound was prepared employing **1a** and **27c** under Suzuki non-migration conditions for 18 h. The reaction mixture was chromatographed using 40:1 hexanes/EtOAc to afford a 93% yield of the indicated compound as a colorless oil: ¹³C NMR (CDCl₃) δ 21.2, 55.2, 113.4, 127.2, 127.4, 128.8, 129.8, 130.6, 130.7, 131.0, 134.2, 136.0, 138.8, 140.2, 140.5, 158.3; all other spectral properties are identical to those previously reported.¹²

Methyl 4''-methoxy-*o*-terphenyl-4-carboxylate (28b). This compound was prepared employing **1b** and **27a** under Suzuki non-migration conditions for 18 h. The reaction mixture was chromatographed using 6:1 hexanes/EtOAc to afford a 92% yield of the indicated compound as a colorless oil, which crystallizes upon cooling and standing: mp 113-114 °C; ¹H NMR (CDCl₃) δ 3.76 (s, 3H), 3.89 (s, 3H), 6.74 (d, *J* = 8.8 Hz, 2H), 7.02 (d, *J* = 8.8 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.41 (m, 4H), 7.90 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (CDCl₃) δ 52.1, 55.2, 113.6, 127.3, 128.1, 128.2, 129.3, 129.9, 130.5, 130.7, 131.0, 133.4, 139.4, 140.3, 146.7, 158.5, 167.2; IR (neat, cm⁻¹) 3024, 2951, 1721; HRMS calcd for C₂₁H₁₈O₃: 318.1256. Found: 318.1261.

Ethyl methyl *o*-terphenyl-4,4''-dicarboxylate (28c). This compound was prepared employing **1c** and **27a** under Suzuki non-migration conditions for 16 h. The reaction mixture was chromatographed using 6:1 hexanes/EtOAc to afford a 98% yield of the indicated

compound as a colorless oil, which crystallizes upon cooling and standing: mp 103-104 °C; ¹H NMR (CDCl₃) δ 1.37 (t, *J* = 7.2 Hz, 3H), 3.89 (s, 3H), 4.35 (q, *J* = 7.2 Hz, 2H), 7.18 (dd, *J* = 2.4, 8.4 Hz, 4H), 7.45 (m, 4H), 7.89 (dd, *J* = 2.0, 8.4 Hz, 4H); ¹³C NMR (CDCl₃) δ 14.4, 52.1, 61.0, 128.28, 128.30, 128.5, 128.8, 129.37, 129.40, 129.87, 129.92, 130.58, 130.60, 139.6, 139.7, 145.8, 145.9, 166.5, 167.0; IR (neat, cm⁻¹) 3024, 2985, 1720; HRMS calcd for C₂₃H₂₀O₄: 360.1362. Found: 360.1371.

Methyl 4''-nitro-*o*-terphenyl-4-carboxylate (28d). This compound was prepared employing **1d** and **27a** under Suzuki non-migration conditions for 5 h. The reaction mixture was chromatographed using 4:1 hexanes/EtOAc to afford a 95% yield of the indicated compound as a colorless solid: mp 149-150 °C; ¹H NMR (CDCl₃) δ 3.90 (s, 3H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 9.0 Hz, 2H), 7.45-7.51 (m, 4H), 7.91 (d, *J* = 8.4 Hz, 2H), 8.07 (d, *J* = 8.7 Hz, 2H); ¹³C NMR (CDCl₃) δ 52.4, 123.6, 128.7, 129.0, 129.1, 129.8, 130.1, 130.6, 130.8, 130.9, 138.5, 139.9, 145.6, 146.8, 148.2, 167.0; IR (neat, cm⁻¹) 3011, 2949, 1722, 1599; HRMS calcd for C₂₀H₁₅NO₄: 333.1001. Found: 333.1007.

2-(4-Methoxycarbonylphenyl)-3-phenylbenzofuran (30). This compound was prepared employing **5** and **27a** under our Suzuki migration conditions for 3 h. The reaction mixture was chromatographed using 9:1 hexanes/EtOAc to afford a 79% yield of the indicated compound as a white solid: mp 122-123 °C; ¹H NMR (CDCl₃) δ 3.90 (s, 3H), 7.23-7.27 (m, 1H), 7.34-7.38 (m, 1H), 7.43-7.51 (m, 6H), 7.56-7.58 (m, 1H), 7.71-7.73 (m, 2H), 7.96-7.98 (m, 2H); ¹³C NMR (CDCl₃) δ 52.2, 111.3, 119.6, 120.4, 123.2, 125.5, 126.6, 128.1, 129.2, 129.4, 129.7, 130.1, 132.4, 134.9, 149.3, 154.2, 166.7 (one sp² carbon missing due to overlap); IR (neat, cm⁻¹) 2917, 2849, 1727; HRMS calcd for C₂₂H₁₆O₃: 328.1099. Found: 328.1104. Anal. calcd for C₂₂H₁₆O₃: C, 80.47; H, 4.91. Found: C, 80.12; H, 4.81.

2-(4-Methoxycarbonylphenyl)-1-methyl-3-phenylindole (32). This compound was prepared employing **9** and **27a** under our Suzuki migration conditions for 3 h. The reaction mixture was chromatographed using 6:1 hexanes/EtOAc to afford a 67% yield of the indicated compound as a white solid: mp 122-123 °C; ¹H NMR (CDCl₃) δ 3.71 (s, 3H), 3.94 (s, 3H), 7.19 (m, 2H), 7.27 (m, 4H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.71 (m, 3H), 7.78 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 2H); ¹³C NMR (CDCl₃) δ 31.2, 52.3, 109.8, 116.2, 119.9, 120.5, 122.8, 125.9, 127.0, 128.4, 129.5, 129.7, 130.0, 131.2, 134.8, 136.5, 136.7, 137.8, 166.9; IR (neat, cm⁻¹) 3053, 2950, 1723; HRMS calcd for C₂₃H₁₉NO₂: 341.1416. Found: 341.1421.

Methyl 5'-methyl-*o*-terphenyl-4-carboxylate (29a). This compound was prepared employing **4a** and **27a** under Suzuki non-migration conditions for 12 h. The reaction mixture was chromatographed using 10:1 hexanes/EtOAc to afford a 90% yield of the indicated compound as a colorless oil: ¹H NMR (CDCl₃) δ 2.42 (s, 3H), 3.86 (s, 3H), 7.07 (m, 2H), 7.14-7.26 (m, 7H), 7.32 (m, 1H), 7.86 (dt, *J* = 8.4, 1.8 Hz, 2H); ¹³C NMR (CDCl₃) δ 21.3, 52.3, 126.8, 128.26, 128.34, 129.1, 129.4, 130.1, 130.2, 130.9, 131.4, 137.6, 138.1, 139.6, 141.2, 146.8, 167.3; IR (neat, cm⁻¹) 3025, 2950, 1727; HRMS calcd for C₂₁H₁₈O₂: 302.1307. Found: 302.1313.

5'-Methyl-*o*-terphenyl. This compound was prepared employing **4a** and **27b** under Suzuki non-migration conditions for 8 h. The reaction mixture was chromatographed using 50:1 hexanes/EtOAc to afford a 93% yield of the indicated compound as a colorless oil. All spectral properties are identical to those previously reported.¹³

4-Methoxy-5'-methyl-*o*-terphenyl. This compound was prepared employing **4a** and **27c** under Suzuki non-migration conditions for 16 h. The reaction mixture was chromatographed using 30:1 hexanes/EtOAc to afford a 94% yield of the indicated

compound as a colorless oil, which crystallizes upon cooling and standing: mp 107-108 °C; ¹H NMR (CDCl₃) δ 2.42 (s, 3H), 3.75 (s, 3H), 6.73 (m, 2H), 7.05 (m, 2H), 7.10-7.22 (m, 7H), 7.30 (d, *J* = 8.4 Hz, 1H); ¹³C NMR (CDCl₃) δ 21.4, 55.4, 113.6, 126.4, 128.1, 130.2, 130.9, 131.2, 131.6, 134.3, 137.4, 137.9, 140.2, 141.9, 158.5 (one sp² carbon missing due to overlap); IR (neat, cm⁻¹) 3026, 2931, 1516; HRMS calcd for C₂₀H₁₈O: 274.1358. Found: 274.1362.

Methyl 5'-methoxy-*o*-terphenyl-4-carboxylate (29b). This compound was prepared employing **4b** and **27a** under Suzuki non-migration conditions for 16 h. The reaction mixture was chromatographed using 6:1 hexanes/EtOAc to afford a 94% yield of the indicated compound as a colorless oil, which crystallizes upon cooling and standing: mp 113-114 °C; ¹H NMR (CDCl₃) δ 3.87 (s, 3H), 3.88 (s, 3H), 6.95-7.01 (m, 2H), 7.02-7.08 (m, 2H), 7.15-7.23 (m, 5H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (CDCl₃) δ 52.3, 55.7, 113.8, 116.0, 126.6, 128.2, 128.5, 129.5, 130.09, 130.14, 132.1, 133.6, 140.9, 141.0, 146.6, 159.2, 167.3; IR (neat, cm⁻¹) 3027, 2951, 1723; HRMS calcd for C₂₁H₁₈O₃: 318.1256. Found: 318.1263.

Ethyl methyl *o*-terphenyl-5',4-dicarboxylate (29c). This compound was prepared employing **4c** and **27a** under Suzuki non-migration conditions for 16 h. The reaction mixture was chromatographed using 5:1 hexanes/EtOAc to afford a 97% yield of the indicated compound as a colorless oil, which crystallizes upon cooling and standing: mp 105-106 °C; ¹H NMR (CDCl₃) δ 1.41 (t, *J* = 7.2 Hz, 3H), 3.89 (s, 3H), 4.42 (q, *J* = 7.2 Hz, 2H), 7.11 (m, 2H), 7.20-7.24 (m, 5H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 8.10 (m, 2H); ¹³C NMR (CDCl₃) δ 14.6, 52.3, 61.4, 127.6, 128.4, 128.8, 129.3, 129.6, 129.9, 130.0, 130.1,

131.1, 131.8, 139.9, 140.3, 145.3, 145.7, 166.5, 167.1; IR (neat, cm^{-1}) 3027, 2983, 1723; HRMS calcd for $\text{C}_{23}\text{H}_{20}\text{O}_4$: 360.1362. Found: 360.1371.

Methyl 5'-nitro-*o*-terphenyl-4-dicarboxylate (29d). This compound was prepared employing **4d** and **27a** under Suzuki non-migration conditions for 5 h. The reaction mixture was chromatographed using 5:1 hexanes/EtOAc to afford an 84% yield of the indicated compound as a colorless solid: mp 124-126 °C; ^1H NMR (CDCl_3) δ 3.91 (s, 3H), 7.10-7.13 (m, 2H), 7.21-7.28 (m, 5H), 7.61 (d, $J = 8.1$ Hz, 1H), 7.93 (dd, $J = 6.6, 1.6$ Hz, 2H), 8.27-8.31 (m, 2H); ^{13}C NMR (CDCl_3) δ 52.4, 123.1, 125.6, 128.3, 128.7, 129.5, 129.7, 129.8, 130.0, 131.9, 139.1, 141.1, 144.2, 147.35, 147.41, 166.9; IR (neat, cm^{-1}) 3063, 2951, 1723, 1611; HRMS calcd for $\text{C}_{20}\text{H}_{15}\text{NO}_4$: 333.1001. Found: 333.1007.

Methyl 4-[2-(benzofuran-3-yl)phenyl]benzoate (31). This compound was prepared employing **8** and **27a** under Suzuki non-migration conditions for 6 h. The reaction mixture was chromatographed using 9:1 hexanes/EtOAc to afford a 75% yield of the indicated compound as a colorless oil: ^1H NMR (CDCl_3) δ 3.87 (s, 3H), 7.11-7.14 (m, 1H), 7.21-7.27 (m, 2H), 7.30-7.34 (m, 3H), 7.42-7.49 (m, 4H), 7.58-7.60 (m, 1H), 7.87-7.89 (m, 2H); ^{13}C NMR (CDCl_3) δ 52.3, 111.7, 120.6, 121.2, 123.0, 124.6, 127.4, 128.3, 128.4, 128.8, 129.5, 129.6, 130.1, 130.8, 131.1, 140.7, 143.1, 146.4, 155.3, 167.2; IR (neat, cm^{-1}) 2973, 2850, 1723; HRMS calcd for $\text{C}_{22}\text{H}_{16}\text{O}_3$: 328.1099. Found: 328.1104.

Methyl 4-[2-(1-methylindol-3-yl)phenyl]benzoate (33). This compound was prepared employing **12** and **27a** under Suzuki non-migration conditions for 16 h. The reaction mixture was chromatographed using 6:1 hexanes/EtOAc to afford a 79% yield of the indicated compound as a white solid: mp 147-148 °C; ^1H NMR (CDCl_3) δ 3.64 (s, 3H), 3.88 (s, 3H), 7.06 (t, $J = 7.2$ Hz, 1H), 7.21 (t, $J = 7.2$ Hz, 1H), 7.28 (d, $J = 8.0$ Hz, 1H), 7.31 (d, J

= 8.0 Hz, 2H), 7.40 (m, 1H), 7.44 (m, 2H), 7.54 (d, $J = 8.0$ Hz, 1H), 7.65 (d, $J = 8.0$ Hz, 1H), 7.85 (d, $J = 8.0$ Hz, 2H); ^{13}C NMR (CDCl_3) δ 32.8, 52.1, 109.3, 114.9, 119.6, 119.9, 121.8, 126.6, 127.2, 128.0, 128.6, 129.2, 129.6, 130.6, 131.3, 133.5, 136.8, 140.0, 147.4, 167.2; IR (neat, cm^{-1}) 3056, 2950, 1719; HRMS calcd for $\text{C}_{23}\text{H}_{19}\text{NO}_2$: 341.1416. Found: 341.1422.

Mass Spectral Data for Deuteration Experiments

Ethyl *E*-3-(biphen-2-yl)acrylate ($\text{C}_{17}\text{H}_{16}\text{O}_2$, nominal mass 252)

^1H NMR (CDCl_3) δ 1.30 (t, $J = 7.1$ Hz, 3H), 2.22 (q, $J = 7.2$ Hz, 2H), 6.43 (d, $J = 15.9$ Hz, 1H), 7.31-7.49 (m, 8H), 7.70-7.79 (m, 2H).

Mass spectral data near 252:

m/z	251	252	253
rel intensity	0	100	18

Deuterated ethyl *E*-3-(biphen-2-yl)acrylate (after synthetic run in D_2O)

^1H NMR (CDCl_3) δ 1.32 (t, $J = 7.1$ Hz, 3H), 2.24 (q, $J = 7.2$ Hz, 2H), 6.45 (d, $J = 15.9$ Hz, 1H), 7.35-7.49 (m, *ca.* 6H), 7.73-7.81 (m, 2H).

^2H NMR (acetone- d_6) δ 7.39 (s)

MS data (FM 252)

m/z	251	252	253	254	255	256
rel intensity	12	30	55	100	90	50

Mass spectral data for 3d (nominal mass 324)

m/z	323	324	325
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intensity	100	30	0
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MS data for 3d, prepared with D₂O

m/z	323	324	325	326	327
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rel intensity	^a	^a	~0	50	100
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^aEdge of noise threshold spanning large *m/z* range, *ca.* 4 relative to 327

Computational Documentation**A simplified computational model, based on naked anions**

As noted in the main text, the data on the equilibrium position of palladation appear to correlate with the C-H acidities of the potential positions. In order to predict this in advance, ideally, high quality calculations could be carried out on a whole series of Pd complexes with appropriate ligands to establish energy differences between the various isomers, instead of the small set we reported in the main text. However, we thought a simplified model, using the relative stabilities of the anions illustrated in Scheme S1, might still provide a qualitative tool if there was a physical basis underlying the apparent correlation. The numbering used in Scheme S1 and in the tables below is consistent with the main text.

Scheme S1.

The energy differences, and, thus, hypothetical equilibrium distributions of the anions, were determined from ΔH and ΔS values as estimated from MP2/6-311+G(d,p)//HF/6-31+G(d) and B3LYP/6-311+G(d,p)//HF/6-31+G(d) total electronic and vibrational calculations. Recognizing the shortcomings of the highly simplified modeling of the anions for the organometallic compounds and the lack of solvation, the originally determined ΔG values were — quite empirically — multiplied by a factor such that the predicted ratio of ions and the product ratio for the Suzuki coupling products of the biphenyl bearing a CO₂Et group would match. It was assumed that solvation/coordination would not be greatly influenced by the substituent, and thus that this correction factor would be approximately constant for a series of related molecules. The adjusted values of ΔG were used to determine the equilibrium constant, K , and subsequently the ratios for the rest of the anions. The results are given in Tables S1 and S2, using MP2/6-311+G(d,p)//RHF/6-31+G(d,p) and B3LYP/6-311+G(d,p)//RHF/6-31+G(d,p) energies, respectively.

Table S1. ΔH , ΔS , ΔG , K, and Calculated Ratios for Substituted Biphenyl and Furan Carbanions Using MP2 Energies.

34, X =	ΔH^a	$T\Delta S^b$	ΔG^b	$\Delta G_{\text{adjusted}}^c$	K_{adjusted}^d	Calc'd 34a:34b ^e	Expt, Heck ^f	Expt, Suzuki ^g
Me	0.14	-0.13	0.27	0.04	0.93	52:48	~50:50	~50:50
NMe ₂	1.04	-0.09	1.13	0.17	0.75	57:43	~48:52	
OMe	1.61	0.10	1.51	0.23	0.68	59:41	~50:50	~60:40
CO ₂ Me	1.91	-0.16	2.07	0.31	0.59	63:37	~55:45	~63:37
OH	2.46	0.20	2.26	0.34	0.56	64:36		
NO ₂	5.37	-0.33	5.70	0.86	0.24	81:19	~64:36	~80:20
Furan ^h	11.61	0.14	11.47	1.72	0.05	95:5	~97:3	~97:3

^a Calculated from the MP2 energies for the forward reaction in Scheme 10 in units of kcal/mol. ^b In kcal/mol, T = 298.15 K. ^c ΔG multiplied by 0.15. ^d Calculated from $\Delta G_{\text{adjusted}}$. ^e From K_{adjusted} . ^f Average of mole ratio of **3:2** from different substrates in Table 2 under “equilibrating” conditions. ^g Average of mol ratio of **29:28** from different substrates in Table 4 under “equilibrating” conditions. ^h Computations using **35**. Heck product ratio of **6** and **7**. Suzuki product ratio of **30** to **31**.

Table S2. ΔH , ΔS , ΔG , K, and Calculated Ratios for Substituted Biphenyl and Furan Carbanions Using B3LYP Energies.

34, X	ΔH^a	$T\Delta S^b$	ΔG^b	$\Delta G_{\text{adjusted}}^c$	K_{adjusted}^d	Calc'd 34a:34b ^e	Expt, Heck ^f	Expt, Suzuki ^g
Me	0.52	-0.13	0.65	0.10	0.85	54:46	~50:50	~50:50
OMe	2.07	0.10	1.97	0.30	0.61	62:48	~50:50	~60:40
CO ₂ Me	0.25	-0.16	0.41	0.06	0.90	53:47	~55:45	~63:37
OH	3.39	0.20	3.19	0.48	0.44	69:31		
NO ₂	2.89	-0.33	3.22	0.48	0.44	69:31	~64:36	~80:20
Furan ^h	13.85	0.14	13.71	2.06	0.03	97:3	~97:3	~97:3

^a Calculated from the MP2 energies for the forward reaction in Scheme 10 in units of kcal/mol. ^b In kcal/mol, T = 298.15 K. ^c ΔG multiplied by 0.15. ^d Calculated from $\Delta G_{\text{adjusted}}$. ^e From K_{adjusted} . ^f Average of mole ratio of **3:2** from different substrates in Table 2 under “equilibrating” conditions. ^g Average of mol ratio of **29:28** from different substrates in Table 4 under “equilibrating” conditions. ^h Computations using **35**. Heck product ratio of **6** and **7**. Suzuki product ratio of **30** to **31**.

The variation between the experimental ratios determined from the Heck and Suzuki procedures is a reminder that the assumption of a rapid equilibrium, followed by precisely identical rates for the product-determining step, is only approximate. Nonetheless, this very

empirical approach to predicting the product ratios for several substituents is surprisingly good, and we take it as support for the general hypothesis of a nearly-equilibrating intermediate, where the favored regiochemistry is determined qualitatively by the acidities of the relevant protons.

Palladium compounds

HF/LANL2DV+ f for Pd, LANL2DV for I, and 6-31G(d) for C,H,P,N

C	6.0	1.5761211741	-.0868267211	-2.6084874285
C	6.0	1.4943746159	-.2022072982	.1771277887
C	6.0	.5423334596	.5129801182	-1.9097870039
C	6.0	2.5808599019	-.7464557370	-1.9195109622
C	6.0	2.5359655339	-.7963032591	-.5399531182
C	6.0	.4804913218	.4661362252	-.5186734499
H	1.0	-.2183790462	1.0394513376	-2.4578302054
H	1.0	3.3960753083	-1.2064296838	-2.4498026151
H	1.0	3.3267754793	-1.2878883059	-.0002526208
PD	46.0	-1.1179094748	1.2953526909	.3985496548
P	15.0	-3.2449582229	2.0189715479	1.5653019488
P	15.0	-2.0226094698	-.8845764202	.7583898914
C	6.0	1.4996185400	-.3127381966	1.6682080116
C	6.0	1.5082538406	-.5512561197	4.5076551351
C	6.0	1.4030646171	.8025396454	2.4947217577
C	6.0	1.6244251623	-1.5449070895	2.3001244374
C	6.0	1.6280110572	-1.6717243716	3.6781608469
C	6.0	1.4076067641	.6931510145	3.8743760679
H	1.0	1.3482370223	1.7818770413	2.0561882241
H	1.0	1.7150136499	-2.4364518712	1.7035424136
H	1.0	1.7256301489	-2.6544122170	4.0950852222
H	1.0	1.3520443370	1.5969877886	4.4472849925
H	1.0	-2.0729534293	-1.8197176463	-.2679743119

C	6.0	-3.8018132114	-.7145297838	1.2656934790
H	1.0	-1.4670095342	-1.6535053892	1.7738622149
H	1.0	-4.2817879169	2.5511877358	.8017439182
H	1.0	-3.2903012626	2.8843900135	2.6527791971
H	1.0	-4.3715349558	-.5386947044	.3576934583
C	6.0	-3.9973205862	.4577149972	2.2456103482
H	1.0	-4.1724980238	-1.6357356383	1.6996304845
H	1.0	-3.4917462360	.2442428818	3.1829653620
H	1.0	-5.0492435363	.5813979349	2.4733329761
I	53.0	-.3044916357	3.8728724148	-.0904952587
N	7.0	1.4736639766	-.6731341346	5.8987854679
H	1.0	1.6014166317	-.0288425025	-3.6828507265
C	6.0	1.9882289124	-1.8931842224	6.4841160369
C	6.0	1.6544265031	.5254716092	6.6898396688
H	1.0	2.6154375867	1.0109646143	6.5192348997
H	1.0	1.5841879035	.2691786253	7.7376276278
H	1.0	.8703331532	1.2426833080	6.4834225765
H	1.0	3.0260070806	-2.0899957620	6.2150928904
H	1.0	1.3923859791	-2.7470450746	6.1864742969
H	1.0	1.9244095473	-1.8218537812	7.5607852712

ZPE = .365175 HARTREE/MOLECULE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ P diffuse + d polarization function, and 6-31G(d) C,H,N,P

C	6.0	1.5754592010	-0.0998559861	-2.6172969998
C	6.0	1.4584559545	-0.1900011920	0.2011682792
C	6.0	0.5130073673	0.4949329537	-1.9318553439
C	6.0	2.5891368886	-0.7383090603	-1.9008061168
C	6.0	2.5260840393	-0.7762770912	-0.5112892290
C	6.0	0.4436234972	0.4581443640	-0.5334079418
H	1.0	-0.2619655301	1.0073318752	-2.4950787550
H	1.0	3.4290436433	-1.1931529296	-2.4206463218
H	1.0	3.3261586741	-1.2519082081	0.0520820761
PD	46.0	-1.2058408499	1.2966668181	0.3549250269
P	15.0	-3.2478610058	2.0725058263	1.3878477567
P	15.0	-2.0150353795	-0.8093502753	0.7930652966
C	6.0	1.4529226171	-0.3114470811	1.6856541357
C	6.0	1.5242609304	-0.5901353566	4.5395576205
C	6.0	1.2458064870	0.7877924940	2.5358371663
C	6.0	1.7007736692	-1.5485311607	2.3005812919
C	6.0	1.7344979059	-1.6950314724	3.6850477669
C	6.0	1.2856995383	0.6587069655	3.9226325611
H	1.0	1.0908667413	1.7732563553	2.1053630565
H	1.0	1.8676098811	-2.4267646227	1.6808828199

H	1.0	1.9341830704	-2.6775816849	4.0956406277
H	1.0	1.1547117458	1.5523160146	4.5217340890
H	1.0	-2.0553420366	-1.8142953164	-0.1977720821
C	6.0	-3.8115842174	-0.6811867724	1.3148633434
H	1.0	-1.4302669516	-1.5555959922	1.8402791520
H	1.0	-4.3022759250	2.5581954517	0.5785117184
H	1.0	-3.3298890692	3.0318325796	2.4216110278
H	1.0	-4.4006307758	-0.6064105391	0.3922412521
C	6.0	-4.0333721666	0.5658298767	2.1922721648
H	1.0	-4.1320366046	-1.5911335174	1.8337867330
H	1.0	-3.5303360647	0.4364123206	3.1585021352
H	1.0	-5.0988300844	0.7163174992	2.3935591373
I	53.0	-0.3632192765	3.8025062796	-0.2099689031
N	7.0	1.5454455002	-0.7306834749	5.9315609204
H	1.0	1.6148380735	-0.0499257447	-3.7035638897
C	6.0	2.0861159372	-1.9609876457	6.4875689701
C	6.0	1.6865448146	0.4663513407	6.7463065779
H	1.0	2.6340044009	1.0026258735	6.5664751366
H	1.0	1.6449615927	0.1879633630	7.8026224251
H	1.0	0.8629795616	1.1632056552	6.5606225579
H	1.0	3.1342220903	-2.1429860719	6.1962995785
H	1.0	1.4903682537	-2.8247328971	6.1715499300
H	1.0	2.0375465276	-1.9174741996	7.5788221174

Energy = -1497.94076 HARTREE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N, 6-31+G(d) for C, H
 Energy = -1498.04939 HARTREE

MP2/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N, 6-31+G(d) for C, H
 Energy = -1494.77161 HARTREE

HF/LANL2DV+ f for Pd, LANL2DV for I, and 6-31G(d) for C,H,P,N

C	6.0	1.44773245	0.25426918	-2.64156342
C	6.0	1.37720633	-0.00700015	0.18075365
C	6.0	0.39459142	0.77061892	-1.87887645
C	6.0	2.46314454	-0.42174131	-1.95432806
C	6.0	2.41698194	-0.53608674	-0.58231890
C	6.0	0.35137579	0.66076261	-0.49407148
H	1.0	-0.40035215	1.29602027	-2.36669183
H	1.0	3.30062604	-0.83969933	-2.47647071
H	1.0	3.22710252	-1.03991890	-0.08339660
Pd	46.0	-1.27924490	1.40157247	0.44400612
P	15.0	-3.43088937	2.02024102	1.62208390
P	15.0	-2.10162306	-0.81977135	0.76036298
C	6.0	1.40311861	-0.18225352	1.66406178
C	6.0	1.45767593	-0.53985649	4.44655800
C	6.0	1.25869775	0.90260822	2.52933455
C	6.0	1.59046054	-1.44546843	2.22550511
C	6.0	1.61818552	-1.62437308	3.59962034
C	6.0	1.28134739	0.72369140	3.90417480
H	1.0	1.15432024	1.89118803	2.12231255
H	1.0	1.70736492	-2.29693675	1.57787740
H	1.0	1.76390064	-2.60994411	4.00642061
H	1.0	1.17984784	1.57780182	4.55057669
H	1.0	-2.12437725	-1.73310375	-0.28633744
C	6.0	-3.88416815	-0.72903663	1.27943861
H	1.0	-1.51044452	-1.59006369	1.75449371
H	1.0	-4.48494625	2.52827930	0.86562324
H	1.0	-3.50758481	2.86418414	2.72440958
H	1.0	-4.46617126	-0.56735557	0.37664020
C	6.0	-4.12582541	0.42126784	2.27492762
H	1.0	-4.21293926	-1.67035627	1.70412898
H	1.0	-3.61488795	0.21354850	3.21063542
H	1.0	-5.18232632	0.50170761	2.50112844
I	53.0	-0.57620537	4.02269983	0.01963981
H	1.0	1.48178446	-0.67542797	5.51338482
N	7.0	1.50186789	0.42002988	-4.02309275
C	6.0	2.32352710	-0.48873413	-4.79189730
C	6.0	0.35875925	0.98589790	-4.70165300
H	1.0	0.59907955	1.11488044	-5.74800825

H	1.0	0.12362382	1.96340621	-4.30202436
H	1.0	-0.53434920	0.36207941	-4.63188124
H	1.0	3.37278247	-0.36694849	-4.55209303
H	1.0	2.20957518	-0.26486143	-5.84323120
H	1.0	2.05781746	-1.53464985	-4.63558626

ZPE = 0.365233 HARTREE/MOLECULE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ P diffuse + d polarization function, and 6-31G(d) C,H,N,P

C	6.0	1.41484833	0.22364886	-2.64665151
C	6.0	1.38282824	-0.02744289	0.20947140
C	6.0	0.37587425	0.77576643	-1.86039269
C	6.0	2.42537332	-0.49031410	-1.96416402
C	6.0	2.40064359	-0.59669781	-0.58057076
C	6.0	0.36032632	0.66600275	-0.47113574
H	1.0	-0.42898706	1.31785798	-2.33979058
H	1.0	3.24581456	-0.94538081	-2.50727034
H	1.0	3.21249652	-1.12492073	-0.08437874
Pd	46.0	-1.30315626	1.41535878	0.47938609
P	15.0	-3.37320518	2.04069185	1.55934536
P	15.0	-2.04044914	-0.74082190	0.75059462
C	6.0	1.41034102	-0.19981304	1.68575191
C	6.0	1.44331646	-0.55567986	4.49137545
C	6.0	1.15358257	0.87699747	2.55537796
C	6.0	1.69800949	-1.45343316	2.25667334
C	6.0	1.71402323	-1.63063037	3.64144182
C	6.0	1.16756392	0.69864845	3.94079494
H	1.0	0.97682571	1.86551034	2.14169765
H	1.0	1.89371049	-2.30099702	1.60429919
H	1.0	1.93354905	-2.61225677	4.05506945
H	1.0	0.98123521	1.55154645	4.58924818
H	1.0	-2.04796171	-1.65866470	-0.32151207
C	6.0	-3.84185410	-0.71742004	1.27416945
H	1.0	-1.43082309	-1.55068469	1.73415911
H	1.0	-4.43925571	2.54615974	0.77795678
H	1.0	-3.49711227	2.91928792	2.65888810
H	1.0	-4.43266153	-0.59582597	0.35768244
C	6.0	-4.10929871	0.45173532	2.24162436
H	1.0	-4.12879896	-1.67431378	1.72298992
H	1.0	-3.60773015	0.26599568	3.19956064
H	1.0	-5.18021727	0.55084515	2.44594669
I	53.0	-0.55039501	3.98203802	0.05632673
H	1.0	1.45855999	-0.69245297	5.56968355
N	7.0	1.45042431	0.39159665	-4.02856779

C	6.0	2.30754876	-0.47414604	-4.82136917
C	6.0	0.31366745	0.99761450	-4.70047665
H	1.0	0.56162524	1.14233410	-5.75539684
H	1.0	0.09472293	1.98257911	-4.27557516
H	1.0	-0.60368448	0.38642254	-4.64093971
H	1.0	3.36130834	-0.34866977	-4.54697704
H	1.0	2.20901179	-0.20202255	-5.87454128
H	1.0	2.05452132	-1.54288220	-4.71522760

Energy = -1497.93652 Hartree

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N, 6-31+G(d) for C, H

Energy = -1498.049164 HARTREE

MP2/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N, 6-31+G(d) for C, H

Energy = -1494.77128 HARTREE

HF/LANL2DV+ f for Pd, LANL2DV for I, and 6-31G(d) for C,H,P,N,O

H	1.0	1.83590925	0.31626487	-5.04355764
C	6.0	1.80174220	0.25801694	-3.96980858
C	6.0	1.68994141	0.13958621	-1.19569504
C	6.0	0.65913779	0.65224576	-3.29577851
C	6.0	2.90216827	-0.19804907	-3.26142812
C	6.0	2.83964443	-0.25563508	-1.88409829
C	6.0	0.57732576	0.60537457	-1.90450597
H	1.0	-0.17540210	1.02196658	-3.86405182
H	1.0	3.79869127	-0.49659562	-3.77463818
H	1.0	3.69663405	-0.59223700	-1.32705629
Pd	46.0	-1.17562175	1.13444316	-1.03465891
P	15.0	-3.41714334	1.51052380	0.04692559
P	15.0	-1.73743927	-1.16637778	-0.69561845

C	6.0	1.69614410	0.03956110	0.29509276
C	6.0	1.69436419	-0.18391101	3.05673003
C	6.0	1.38031757	1.13712621	1.09746075
C	6.0	2.03396344	-1.16407204	0.91646940
C	6.0	2.03413558	-1.28573275	2.29282093
C	6.0	1.37606728	1.03143311	2.47629666
H	1.0	1.15586042	2.08097935	0.63913387
H	1.0	2.28769588	-2.01675677	0.31358474
H	1.0	2.28499603	-2.21218538	2.76857734
H	1.0	1.14072049	1.87586975	3.09227014
N	7.0	1.67108226	-0.30886975	4.50624275
H	1.0	-1.61102438	-2.09128666	-1.72431076
C	6.0	-3.53317308	-1.27836967	-0.23185147
H	1.0	-1.09042239	-1.84494352	0.33127633
H	1.0	-4.49243927	1.87399006	-0.75982362
H	1.0	-3.62047982	2.37123609	1.11885953
H	1.0	-4.09990931	-1.20953548	-1.15586972
C	6.0	-3.94124818	-0.14170122	0.72407663
H	1.0	-3.75938201	-2.24230433	0.20846392
H	1.0	-3.44292402	-0.26486653	1.68126857
H	1.0	-5.00695753	-0.18089488	0.91449648
I	53.0	-0.76935738	3.80298257	-1.47910476
O	8.0	1.36202645	0.65255523	5.14363480
O	8.0	1.95435488	-1.36983120	4.97817564

ZPE = .290601 HARTREE/MOLECULE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ P diffuse + d polarization function, and 6-31G(d) C,H,N,P,O

H	1.0	1.84882796	0.28833732	-5.08015442
C	6.0	1.80438209	0.23967749	-3.99430704
C	6.0	1.66819501	0.14923745	-1.18715119
C	6.0	0.64108288	0.63483942	-3.32901263
C	6.0	2.90922070	-0.20076497	-3.26297927
C	6.0	2.83488107	-0.24462062	-1.87513125
C	6.0	0.55624801	0.59919101	-1.93070793
H	1.0	-0.20475151	0.99310315	-3.90922666
H	1.0	3.82319403	-0.49996325	-3.76949072
H	1.0	3.69984889	-0.56666166	-1.29936147
Pd	46.0	-1.22794557	1.11059797	-1.05530894
P	15.0	-3.35907125	1.54466963	-0.02077933
P	15.0	-1.74135005	-1.11565423	-0.71420139
C	6.0	1.66762626	0.04177174	0.29692084
C	6.0	1.69399559	-0.22359370	3.07956934
C	6.0	1.23989320	1.09943175	1.12411964
C	6.0	2.12291312	-1.14246631	0.90870631

C	6.0	2.13815308	-1.28569317	2.29182315
C	6.0	1.25166428	0.97157735	2.51171374
H	1.0	0.92666954	2.03866625	0.67822975
H	1.0	2.45356178	-1.96866286	0.28583366
H	1.0	2.47830224	-2.19866037	2.76578498
H	1.0	0.93865883	1.78554285	3.15468335
N	7.0	1.69504166	-0.36985409	4.53990459
H	1.0	-1.65532565	-2.06374621	-1.75617886
C	6.0	-3.53420758	-1.25241303	-0.18407196
H	1.0	-1.04632008	-1.82856166	0.28836781
H	1.0	-4.46186829	1.91462362	-0.82518446
H	1.0	-3.55464840	2.45720387	1.03797936
H	1.0	-4.13242006	-1.23401403	-1.10361302
C	6.0	-3.92766666	-0.07802179	0.73202080
H	1.0	-3.72232080	-2.21376014	0.30569547
H	1.0	-3.41443586	-0.16683921	1.69728482
H	1.0	-5.00405979	-0.08398663	0.93028605
I	53.0	-0.79172438	3.72674036	-1.55450487
O	8.0	1.28295648	0.57665920	5.21274137
O	8.0	2.10279822	-1.43393266	5.00970030

Energy = -1568.48222 HARTREE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N& O, 6-31+G(d) for C, H

Energy = -1568.64625 HARTREE

MP2/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N& O, 6-31+G(d) for C, H
Energy = -1565.39048 HARTREE

HF/LANL2DV+ f for Pd, LANL2DV for I, and 6-31G(d) for C,H,P,N,O

N	7.0	1.87952793	0.31807858	-4.77727938
C	6.0	1.82459283	0.25905609	-3.32140255

C	6.0	1.68870652	0.11257151	-0.57708889
C	6.0	0.66495848	0.64262748	-2.67654395
C	6.0	2.93750286	-0.18351431	-2.63036704
C	6.0	2.85413337	-0.25362638	-1.25723207
C	6.0	0.57646531	0.57770073	-1.28828573
H	1.0	-0.15703757	0.99962264	-3.26306987
H	1.0	3.83013701	-0.45895341	-3.15378714
H	1.0	3.70895600	-0.58476299	-0.69612616
Pd	46.0	-1.17857504	1.10075486	-0.41100559
P	15.0	-3.40291333	1.49562716	0.65940362
P	15.0	-1.76317871	-1.19743586	-0.08562494
C	6.0	1.67116249	-0.02642692	0.91266620
C	6.0	1.63798940	-0.32156527	3.69382644
C	6.0	1.36460960	1.05356824	1.73813891
C	6.0	1.97650445	-1.24995518	1.50535595
C	6.0	1.95581019	-1.39917076	2.88311005
C	6.0	1.34866250	0.90499055	3.11657596
H	1.0	1.16025984	2.01336861	1.30180550
H	1.0	2.22415996	-2.09231853	0.88326627
H	1.0	2.19069409	-2.35346293	3.32048106
H	1.0	1.12282932	1.75340950	3.73778009
H	1.0	-1.64128244	-2.12206244	-1.11522079
C	6.0	-3.56326389	-1.28804660	0.36597028
H	1.0	-1.12879360	-1.88131666	0.94502455
H	1.0	-4.46078014	1.88361061	-0.15807471
H	1.0	-3.59534073	2.35745263	1.73213637
H	1.0	-4.12367392	-1.20781982	-0.56085628
C	6.0	-3.96129632	-0.14971064	1.32433319
H	1.0	-3.80476975	-2.25095081	0.80030191
H	1.0	-3.47316837	-0.28594047	2.28503251
H	1.0	-5.02916813	-0.17051524	1.50509131
I	53.0	-0.76402712	3.76871490	-0.83196586
H	1.0	1.62751293	-0.43328258	4.76340914
O	8.0	2.92690158	0.08462854	-5.30383301
O	8.0	0.87518418	0.58505493	-5.36594534

ZPE = .290494 HARTREE/MOLECULE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ P diffuse + d polarization function, and 6-31G(d) C,H,N,P,O

N	7.0	1.88150203	0.29587021	-4.80446672
C	6.0	1.81862533	0.24828310	-3.33589220
C	6.0	1.66785121	0.12117074	-0.55857420
C	6.0	0.64352316	0.63855755	-2.69434738
C	6.0	2.93547702	-0.19048598	-2.62694812

C	6.0	2.84457707	-0.24906917	-1.24341869
C	6.0	0.55657977	0.58206183	-1.29968464
H	1.0	-0.18608323	0.98816043	-3.29657722
H	1.0	3.83805728	-0.47028559	-3.15626931
H	1.0	3.70600843	-0.57595527	-0.66669005
Pd	46.0	-1.22523022	1.08550656	-0.41311386
P	15.0	-3.34660697	1.51670408	0.62057340
P	15.0	-1.76126659	-1.14319122	-0.12677138
C	6.0	1.64723754	-0.02641483	0.92445856
C	6.0	1.63930130	-0.35538608	3.72368264
C	6.0	1.24969208	1.02596498	1.76764953
C	6.0	2.04994416	-1.23930168	1.50952446
C	6.0	2.04165697	-1.40559912	2.89532518
C	6.0	1.24988091	0.85992831	3.15515733
H	1.0	0.97503895	1.98501885	1.33824503
H	1.0	2.36032057	-2.06197548	0.86999995
H	1.0	2.35266209	-2.35431099	3.32562709
H	1.0	0.95801598	1.69206703	3.79089856
H	1.0	-1.67722762	-2.07217407	-1.18586695
C	6.0	-3.55738497	-1.27302873	0.39223185
H	1.0	-1.07441294	-1.87491894	0.86707717
H	1.0	-4.43656063	1.91994822	-0.18450722
H	1.0	-3.53443408	2.40946794	1.69723153
H	1.0	-4.15124273	-1.22824693	-0.52900660
C	6.0	-3.94102192	-0.11492360	1.33307719
H	1.0	-3.75748205	-2.24259567	0.86040622
H	1.0	-3.43354368	-0.23270389	2.29828048
H	1.0	-5.01857233	-0.11093161	1.52486980
I	53.0	-0.77029771	3.71386194	-0.81516892
H	1.0	1.64189863	-0.48019639	4.80337238
O	8.0	2.94819808	-0.00789135	-5.34282064
O	8.0	0.86531031	0.62701499	-5.41756392

Energy = -1568.48284 HARTREE

B3LYP/ LANL2DV+ f for Pd, LANL2DV for I+ S & P diffuse + d & F polarization function, and 6-31G+G(3df) for P, 6-311+G(2d) for N& O, 6-31+G(d) for C, H

Energy = -1568.64722 HARTREE

Anions

2-carbanion of 4-hydroxybiphenyl

HF/6-31+G(d,p)

C	6.0	.0610065004	.0241960470	-.9372952832
C	6.0	.0928247308	.0348147732	.5586221194
C	6.0	.0379155870	.0464054185	3.3223186319
C	6.0	1.2974712792	.3965322291	1.2239099218
C	6.0	-1.0632448588	-.3257591675	1.2532353563
C	6.0	-1.1101153256	-.3249900718	2.6415973089
C	6.0	1.1898607292	.3868006948	2.6274184516
H	1.0	-1.9479997499	-.6411414182	.7217349121
H	1.0	-1.9958923221	-.6138596390	3.1810325419
H	1.0	2.0573319721	.6567142584	3.2255654640
O	8.0	-.0048693711	.0521642572	4.6950216524
C	6.0	.0450437428	-.0367767726	-3.7678628446
C	6.0	-1.0973317767	.2973049648	-1.6723750277
C	6.0	1.2205837320	-.2614992413	-1.6715550427
C	6.0	1.2122323873	-.2951725707	-3.0551744701
C	6.0	-1.1086272086	.2638198480	-3.0619113738
H	1.0	-2.0014456235	.5660429340	-1.1555604358
H	1.0	2.1259846993	-.4424418786	-1.1253437020
H	1.0	2.1228070674	-.5245114188	-3.5847986501
H	1.0	-2.0215370255	.4866976664	-3.5902917934
H	1.0	.0408236203	-.0603531836	-4.8448884374
H	1.0	.8457692861	.3138300921	5.0182088693

Energy	-534.4802491009 Hartree
ZPE	.183084 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-536.4717137938 Hartree
B3LYP/6-311+G(d,p)	-537.7079700998 Hartree

2'-carbanion of 4-hydroxybiphenyl

HF/6-31+G(d,p)

C	6.0	.0460082284	.0580955637	-.4315921461
C	6.0	.0757371982	.0690723435	1.0688274136
C	6.0	.0179896902	.0631129537	3.8359843438
C	6.0	1.1473677147	.7273890477	1.7253041128
C	6.0	-.9547638296	-.5847291673	1.7553579613
C	6.0	-.9950416660	-.5898962185	3.1423011924
C	6.0	1.0448998765	.6852965303	3.1340226209
H	1.0	-1.7247882686	-1.1164693694	1.2166815492

H	1.0	-1.7885631143	-1.1000677544	3.6657322220
H	1.0	1.8154846394	1.1677953059	3.7232644160
H	1.0	.0078900351	.0745151925	4.9171463339
C	6.0	.0498429248	.0267156206	-3.2558906994
C	6.0	-1.1361490872	.0407663425	-1.1735477144
C	6.0	1.2354781560	.0779594527	-1.1640208173
C	6.0	1.2435438304	.0579212735	-2.5502492808
C	6.0	-1.1451780722	.0221661967	-2.5642568973
H	1.0	-2.0820044217	.0665368580	-.6625350827
H	1.0	2.1583199141	.1239956122	-.6189744509
H	1.0	2.1843548796	.0675658114	-3.0806571728
H	1.0	-2.0724192104	.0173263697	-3.1106774506
O	8.0	.0121251448	.0064938319	-4.6258793934
C	1.0	.8930696008	.0502783260	-4.9684917752

Energy	-534.4735035275 Hartree
ZPE	.182774 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-536.4674726383
B3LYP/6-311+G(d,p)	-537.7022560781

2-carbanion of 4-nitrobiphenyl

HF/6-31+G(d,p)

C	6.0	-0.0017277833	-0.1428960045	-0.3140383338
C	6.0	-0.0125682442	-0.1036462691	1.1848109358
C	6.0	0.0011204135	-0.0691952787	4.0044763099
C	6.0	0.5075114763	-1.1731988401	1.9212991453
C	6.0	-0.5393571361	0.9719842457	1.9023464206
C	6.0	-0.5340757290	0.9915633038	3.2919722029
C	6.0	0.5202128057	-1.1538645370	3.3056762985
C	1.0	0.8857312188	-2.0191008204	1.3809324217
H	1.0	-0.9849219629	1.7962353343	1.3745774793
H	1.0	-0.9586230112	1.8335280812	3.8133700264
H	1.0	0.9331277511	-1.9907522170	3.8441691171
H	1.0	0.0068182775	-0.0578324090	5.0814162406
C	6.0	-0.0181822892	-0.0902641996	-3.0485623260
C	6.0	0.1463814602	1.0746159330	-1.0014622479
C	6.0	-0.1303600861	-1.3926928540	-0.9603127402
C	6.0	-0.1362006339	-1.2947830010	-2.3702050685
C	6.0	0.1369073371	1.1184819090	-2.3787740908
H	1.0	0.2937509928	1.9972779345	-0.4646654480
H	1.0	-0.2366875599	-2.1875301013	-2.9603515846
H	1.0	0.2546247171	2.0388440560	-2.9148626018
N	7.0	-0.0384755303	-0.0675622226	-4.5059799772
O	8.0	0.0591629675	0.9942442451	-5.0650981513
O	8.0	-0.1516275505	-1.1026337854	-5.1006399588

Energy	-663.1195003069 Hartree
ZPE	.182401 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-665.5185312616
B3LYP/6-311+G(d,p)	-666.9900726504

2'-carbanion of 4-nitrobiphenyl

HF/6-31+G(d,p)

C	6.0	0.0469790907	-0.0839666425	-0.1865668558
C	6.0	0.0453594275	-0.1161833850	1.3020413278
C	6.0	0.0526405396	-0.0749364609	4.0639385268
C	6.0	0.5329568334	-1.2781198578	1.9490177644
C	6.0	-0.4441280122	1.0047840003	1.9952295340
C	6.0	-0.4470328172	1.0323142041	3.3761567922
C	6.0	0.5153574160	-1.1759065499	3.3621400582
H	1.0	-0.8528667324	1.8502971295	1.4648556695
H	1.0	-0.8363400879	1.8859091912	3.9071576644
H	1.0	0.8798756901	-2.0120382897	3.9448049768
H	1.0	0.0657691442	-0.0703574874	5.1445529240
C	6.0	0.0235592153	-0.0828376078	-2.9886645809
C	6.0	0.1082391223	1.1109296628	-0.9231260185
C	6.0	-0.0039714295	-1.2835608852	-0.9204044926
C	6.0	-0.0212467938	-1.2905746454	-2.2960645374
C	6.0	0.0947792184	1.1202075374	-2.3037137638
H	1.0	0.1956319125	2.0496293982	-0.4099987949
H	1.0	-0.0182009162	-2.2021246792	-0.3690762433
H	1.0	-0.0707221250	-2.2148110580	-2.8374019567
H	1.0	0.1482047908	2.0435698565	-2.8459866528
N	7.0	0.0044329290	-0.0801533808	-4.4300314259
O	8.0	0.0475996138	0.9766454664	-5.0020105802
O	8.0	-0.0553751634	-1.1336153606	-5.0035633742

Energy	-663.1136120824 Hartree
ZPE	.182270 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-665.5098445646
B3LYP/6-311+G(d,p)	-666.9853352878

2-carbanion of 4-carbomethoxybiphenyl

HF/6-31+G(d,p)

C	6.0	-0.1577064373	-0.2911845642	-3.5432563557
C	6.0	-0.1238987676	-0.2585133169	-2.0631907882
C	6.0	-0.1215239358	-0.2918118353	0.7044177610
C	6.0	-0.6244782431	-1.3429924278	-1.3437527572

C	6.0	0.4137052739	0.8335022439	-1.3738970913
C	6.0	0.4121706940	0.8047268758	0.0044858436
C	6.0	-0.6533143386	-1.4349126839	0.0673685263
H	1.0	-1.0137728558	-2.1631879056	-1.9247024960
H	1.0	0.8291957292	1.6713081035	-1.9024522319
H	1.0	0.8532444731	1.6339583094	0.5343613924
C	6.0	-0.1087211139	-0.2402951718	2.2033282681
C	6.0	-0.0511509141	-0.1955208644	5.0257156565
C	6.0	0.0227894119	-1.4183567590	2.9478250363
C	6.0	-0.2304217938	0.9541070970	2.9172593093
C	6.0	-0.2013420008	0.9791470926	4.3068079921
C	6.0	0.0573120552	-1.3963017536	4.3316570291
H	1.0	0.0831946228	-2.3450836949	2.4110599611
H	1.0	-0.3744908341	1.8779091647	2.3861021002
H	1.0	-0.3052083075	1.9190363930	4.8238338169
H	1.0	0.1673068348	-2.3207581467	4.8744944407
H	1.0	-0.0266942850	-0.1801047533	6.1024839547
O	8.0	-0.5727061683	-1.1861320390	-4.2229485080
O	8.0	0.3376613084	0.8189100185	-4.1142721602
C	6.0	0.3377465870	0.8669344869	-5.5183645552
H	1.0	0.9343702380	0.0659408174	-5.9346994751
H	1.0	0.7668615064	1.8238670531	-5.7824309203
H	1.0	-0.6683793133	0.7915252817	-5.9092839723

Energy -686.2775067761Hartree
ZPE .225330 HARTREE/MOLECULE
MP2/6-311+G(d,p) -688.7748585834
B3LYP/6-311+G(d,p) -690.3305591927

2'-carbanion of 4-carbomethoxybiphenyl

HF/6-31+G(d,p)

C	6.0	-0.1183198009	-0.2947069393	-3.4810901031
C	6.0	-0.0854320501	-0.2533662690	-2.0077952525
C	6.0	-0.0583626138	-0.2551167106	0.8231013331
C	6.0	-0.5487553821	-1.3564191767	-1.2842089875
C	6.0	0.4015060257	0.8426062536	-1.3005599817
C	6.0	0.4141674972	0.8381348959	0.0825419934
C	6.0	-0.5308939313	-1.3590010018	0.0935560793
H	1.0	-0.9221177466	-2.2101067145	-1.8199855303
H	1.0	0.7811879582	1.6956649129	-1.8314693444
H	1.0	0.8251872557	1.6888763916	0.5939890522
H	1.0	-0.8670945634	-2.2142952381	0.6453760126
C	6.0	-0.0592246181	-0.2775164676	2.3160192973
C	6.0	-0.0121283981	-0.2134356742	5.0794127506
C	6.0	0.0481587968	-1.5279029121	2.9746309073

C	6.0	-0.1679032225	0.9444838289	2.9991932029
C	6.0	-0.1465151787	0.9862488056	4.3817626793
C	6.0	0.0754655933	-1.4112311490	4.3857047557
H	1.0	-0.2966086052	1.8698202551	2.4596290737
H	1.0	-0.2419531016	1.9248525602	4.9041774094
H	1.0	0.1650814461	-2.3140320959	4.9767834322
H	1.0	0.0119804150	-0.2036927947	6.1601458212
O	8.0	-0.5242376520	-1.2088303881	-4.1410731739
O	8.0	0.3591965002	0.8136362282	-4.0565563873
C	6.0	0.3664540255	0.8516468093	-5.4643249758
H	1.0	0.9754250706	0.0540337955	-5.8677047095
H	1.0	0.7858070282	1.8111025246	-5.7312231284
H	1.0	-0.6371441511	0.7622167673	-5.8573794091
Energy				-686.2772911244 Hartree
ZPE				.225243 HARTREE/MOLECULE
MP2/6-311+G(d,p)				-688.7717373018
B3LYP/6-311+G(d,p)				-690.3300872560

2-carbanion of 4-methylbiphenyl

HF/6-31+G(d,p)

C	6.0	-.1063369181	.0822295899	-.1042357837
C	6.0	-.0693746807	.0695476248	1.3929007430
C	6.0	-.0555124976	.0305731833	4.2219199006
C	6.0	-1.2423842162	.2676149955	2.1337031139
C	6.0	1.1091743491	-.1282876862	2.1187538426
C	6.0	1.1181715045	-.1511875214	3.5087354638
C	6.0	-1.2366313696	.2445892408	3.5175073284
H	1.0	-2.1495354847	.4525384903	1.5917334776
H	1.0	2.0412076943	-.2412525845	1.5941830677
H	1.0	2.0491086121	-.3006008041	4.0314909048
H	1.0	-2.1594684818	.3949675861	4.0539286486
H	1.0	-.0525288370	.0150296502	5.2991051086
C	6.0	-.0637874786	.0581094570	-2.8933035572
C	6.0	.8075136868	-.7210656874	-.7986017933
C	6.0	-1.0637653929	.8904207657	-.7637827918
C	6.0	-.9719876951	.8278342174	-2.1746367307
C	6.0	.8359726006	-.7379606430	-2.1827134338
H	1.0	1.4917742541	-1.3642260437	-.2659792071
H	1.0	-1.6659137522	1.4236343143	-2.7567849127
H	1.0	1.5399508810	-1.3711261525	-2.7024179080
C	6.0	-.0432375868	.0636403487	-4.4076935291
H	1.0	.9002435625	.4455763908	-4.7949033053
H	1.0	-.8386309174	.6873897045	-4.8047514798
H	1.0	-.1740218362	-.9379884915	-4.8141569012

Energy	-498.6526973189 Hartree
ZPE	.207478 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-500.5827198937 Hartree
B3LYP/6-311+G(d,p)	-501.7833436215 Hartree

2'-carbanion of 4-methylbiphenyl

HF/6-31+G(d,p)

C	6.0	.0076116966	.0977577973	.0185206365
C	6.0	.0316908323	.1244415772	1.5172765226
C	6.0	.0114902639	.0745633767	4.2840304805
C	6.0	-.3114541041	-1.0480456167	2.2032018634
C	6.0	.4100499770	1.3235619331	2.1739886139
C	6.0	.3690045675	1.2207106374	3.5835943096
C	6.0	-.3270237906	-1.0826396351	3.5893941431
H	1.0	-.5465291750	-1.9526439193	1.6629494136
H	1.0	.6360334671	2.0894781050	4.1732981115
H	1.0	-.5846106575	-1.9904284897	4.1122542198
H	1.0	.0047880452	.0730726280	5.3653406385
C	6.0	.0280541961	.0663242473	-2.8307723076
C	6.0	.8943361654	.8930162759	-.7216603693
C	6.0	-.8748376763	-.6921614561	-.7153256835
C	6.0	-.8624013253	-.7105333691	-2.1086429962
C	6.0	.9057168456	.8728849485	-2.1031427571
H	1.0	1.5627684954	1.5330217490	-.1789389651
H	1.0	-1.6049989164	-1.2918819736	-.2012884989
H	1.0	-1.5692408547	-1.3370443255	-2.6300938259
H	1.0	1.6109283553	1.4970835319	-2.6306783125
C	6.0	.0480483749	.0607917722	-4.3431247229
H	1.0	1.0346456570	-.1868115952	-4.7282084658
H	1.0	-.2219945519	1.0328378300	-4.7501116401
H	1.0	-.6520757305	-.6673560287	-4.7418602505

Energy	-498.6521092969 Hartree
ZPE	.207526 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-500.5825429295 Hartree
B3LYP/6-311+G(d,p)	-501.7825620739 Hartree

2'-carbanion of 4-N,N-dimethylaminobiphenyl

HF/6-31+G(d,p)

C	6.0	0.0407120584	0.7577982457	-0.4965067689
C	6.0	-0.0710715347	2.0565351819	-1.2365951211
C	6.0	-0.1576188284	4.4514274954	-2.6193398249

C	6.0	1.0539897996	2.8903699395	-1.2817405385
C	6.0	-1.3056057454	2.3865621808	-1.8519133119
C	6.0	-1.2681812132	3.6195155836	-2.5432577028
C	6.0	1.0213813100	4.0915883251	-1.9733617075
H	1.0	1.9589786889	2.6221454185	-0.7578763079
H	1.0	-2.1633823886	3.9535943210	-3.0537158245
H	1.0	1.8877710675	4.7337038070	-1.9978987737
H	1.0	-0.2072065877	5.3814631292	-3.1686959605
C	6.0	0.1936993454	-1.7023428695	0.9120414458
C	6.0	-1.0773639526	0.2063094122	0.1429511782
C	6.0	1.2280563027	0.0295303783	-0.4132505141
C	6.0	1.3048655535	-1.1758236260	0.2783909459
C	6.0	-1.0024786337	-0.9898062681	0.8334147900
H	1.0	-2.0080715547	0.7343606243	0.0671301706
H	1.0	2.1073741186	0.3877261116	-0.9183292884
H	1.0	2.2322608895	-1.7219888564	0.3160467913
H	1.0	-1.8884860252	-1.3735638073	1.3125208337
N	7.0	0.3068042596	-2.9584610929	1.6054954646
C	6.0	-0.4673936547	-4.0272016117	1.0085630997
C	6.0	0.0996373349	-2.8634906282	3.0352451070
H	1.0	-0.9351643201	-2.6409797283	3.3110197580
H	1.0	0.7315915557	-2.0848273300	3.4434944176
H	1.0	0.3733600601	-3.8059495217	3.5029184272
H	1.0	-1.5471706042	-3.8990226213	1.1256694185
H	1.0	-0.1918372753	-4.9732308967	1.4678716024
H	1.0	-0.2494439399	-4.0859399219	-0.0502940821

Energy -592.6949562409 Hartree
ZPE .256300 HARTREE/MOLECULE
MP2/6-311+G(d,p) -594.8826958823 Hartree

2-carbanion of 4-N,N-dimethylaminobiphenyl

HF/6-31+G(d,p)

C	6.0	.0178689151	.7458215208	-.3106767088
C	6.0	-.0404049517	2.0068408063	-1.1159288577
C	6.0	-.1639084781	4.4185547860	-2.5924067076
C	6.0	.5407235757	2.1235107101	-2.3825278863
C	6.0	-.7040631853	3.1372254451	-.6193294649
C	6.0	-.7618127734	4.3177141149	-1.3396135990
C	6.0	.4841115454	3.3079412856	-3.1082738977
H	1.0	1.0239881624	1.2703212393	-2.8243960026
H	1.0	-1.1815782069	3.0552767768	.3377598115
H	1.0	-1.2779676443	5.1675249832	-.9230823198
H	1.0	.9381904737	3.3536335263	-4.0849323747
H	1.0	-.2119946125	5.3375009137	-3.1528322419

C	6.0	.1973827970	-1.6487506966	1.1013216717
C	6.0	-1.0416264646	.4457088147	.5788082782
C	6.0	1.1306653937	-.0918399441	-.4600783272
C	6.0	1.2304810339	-1.2815640193	.2391791214
C	6.0	-.8847360699	-.7893377301	1.2534648757
H	1.0	1.9540052184	.1925211801	-1.0978418458
H	1.0	2.1041020241	-1.9062434619	.1477810841
H	1.0	-1.6629314073	-1.0858172699	1.9416156609
N	7.0	.3193892012	-2.9076007150	1.7899025536
C	6.0	-.0142912258	-4.0505562237	.9660476494
C	6.0	-.3101488050	-2.9889052737	3.0865556371
H	1.0	-1.0837534191	-4.1048843880	.7377541898
H	1.0	.2695260352	-4.9666601112	1.4799034320
H	1.0	.5251570396	-4.0059615449	.0293965189
H	1.0	-1.4003785936	-3.0593101491	3.0442073782
H	1.0	-.0518369610	-2.1185276489	3.6756562769
H	1.0	.0558296360	-3.8741023727	3.6025529698
Energy -592.6964352805 Hartree				
ZPE .256519 HARTREE/MOLECULE				
MP2/6-311+G(d,p) -594.8845659066 Hartree				

2-carbanion of 4-methoxybiphenyl

HF/6-31+G(d,p)

C	6.0	-.0799082731	-.0041936655	.1411309792
C	6.0	-.1651548995	.0278475992	1.6341684591
C	6.0	-.2814720875	.0409774437	4.4631026280
C	6.0	.9631265776	-.2571216396	2.4162643760
C	6.0	-1.3437344131	.3388353434	2.3203327461
C	6.0	-1.4041715914	.3419423355	3.7091839261
C	6.0	.9056491866	-.2542048345	3.7988607141
H	1.0	1.8832075413	-.4679148156	1.9064136895
H	1.0	-2.2250102586	.6072220874	1.7651359674
H	1.0	-2.3313359072	.5923163503	4.1990959910
H	1.0	1.7929829822	-.4847832893	4.3660065275
H	1.0	-.3241658186	.0435833337	5.5396182741
C	6.0	-.0281460439	-.0768763748	-2.6295351646
C	6.0	-1.2206129654	-.3616082140	-.5872228478
C	6.0	1.1489751724	.3112981091	-.4890368467
C	6.0	1.1039138050	.2630815379	-1.9034372883
C	6.0	-1.2101256470	-.4017825868	-1.9698924844
H	1.0	-2.1325177916	-.6415685698	-.0820941501
H	1.0	2.0061005434	.5022676871	-2.4441210541
H	1.0	-2.0791155456	-.6892787694	-2.5367188485
O	8.0	-.0890844518	-.1347875269	-4.0001944706

C	6.0	1.0560573875	.1267511261	-4.7423041597
H	1.0	1.8605135375	-.5610159700	-4.4977693717
H	1.0	1.4099346815	1.1431064523	-4.5938944727
H	1.0	.7835528263	-.0035309024	-5.7830142718
Energy				-573.5017480223 Hartree
ZPE				.213691 HARTREE/MOLECULE
MP2/6-311+G(d,p)				-575.6465054722 Hartree
B3LYP/6-311+G(d,p)				-576.9849017274 Hartree

2'-carbanion of 4-methoxybiphenyl

HF/6-31+G(d,p)

C	6.0	.0213868346	.2852071533	-.0884270135
C	6.0	-.3525364857	1.3636848207	-1.0616882619
C	6.0	-.9275320344	3.3834209992	-2.8638632842
C	6.0	.6727330458	1.9713713161	-1.7966423786
C	6.0	-1.7206183872	1.7101978029	-1.2070107680
C	6.0	-1.9322172350	2.7512744314	-2.1389557975
C	6.0	.3951843593	2.9864477918	-2.7010413240
H	1.0	1.6957922006	1.6428526422	-1.6893328517
H	1.0	-2.9460064919	3.0915035068	-2.3128322383
H	1.0	1.1882027345	3.4452666057	-3.2706173671
H	1.0	-1.1694038590	4.1740963274	-3.5607506152
C	6.0	.6874710999	-1.7850591763	1.7231223209
C	6.0	1.2246101007	.2842322298	.6250474451
C	6.0	-.8391710765	-.7815075673	.1579263453
C	6.0	-.5205941787	-1.8071054406	1.0419030124
C	6.0	1.5587089588	-.7271637154	1.5117344404
H	1.0	1.9114279082	1.1033303371	.5059679976
H	1.0	-1.7837035837	-.7913253804	-.3508748510
H	1.0	-1.2256539825	-2.6055252845	1.1837890341
H	1.0	2.4870970552	-.7002506563	2.0554593528
O	8.0	1.0932136883	-2.7402971002	2.6138078654
C	6.0	.2730093022	-3.8389311213	2.8489158835
H	1.0	-.6883033815	-3.5424515625	3.2590762378
H	1.0	.7883928917	-4.4570317858	3.5722033914
H	1.0	.1076182943	-4.4162154028	1.9431272253
Energy				-573.4969209563 Hartree
ZPE				.213560 HARTREE/MOLECULE
MP2/6-311+G(d,p)				-575.6438026917 Hartree
B3LYP/6-311+G(d,p)				-576.9814497925 Hartree

2'-carbanion of 3-phenylfuran

HF/6-31+G(d,p)

C	6.0	0.0158217274	0.1737512269	-1.2228674365
C	6.0	0.0148402356	-0.2817281743	0.1936669993
C	6.0	0.0003403249	-1.0386613434	2.8516954665
C	6.0	0.0360513585	-1.6791791649	0.4514400721
C	6.0	-0.0054731373	0.6845826111	1.2017289990
C	6.0	-0.0148094353	0.3145102430	2.5413116187
C	6.0	0.0279404425	-1.9844138781	1.8282739212
H	1.0	-0.0114187495	1.7370081068	0.9596334250
H	1.0	-0.0320941688	1.0641227562	3.3168749803
H	1.0	0.0423161803	-3.0253031996	2.1289297100
H	1.0	-0.0082237539	-1.3522584872	3.8865332817
C	6.0	0.1261014607	-0.5992970729	-2.3197146772
C	6.0	-0.1076831895	1.5214344534	-1.7514782230
H	1.0	0.2319467353	-1.6534655265	-2.4335048071
O	8.0	0.0827521734	0.1390952096	-3.4622942968
C	6.0	-0.0601390556	1.4182547103	-3.0881844452
H	1.0	-0.2224508473	2.4332610101	-1.2012936998
H	1.0	-0.1171978126	2.1414840327	-3.8746446081

Energy	-457.5407665136 Hartree
ZPE	0.146540 HARTREE/MOLECULE
MP2/6-311+G(d,p)	-459.2298829273 Hartree
B3LYP/6-311+G(d,p)	-460.2831012574 Hartree

2-carbanion of 3-phenylfuran

HF/6-31+G(d,p)

C	6.0	.0180454368	.1501180132	-1.3755640486
C	6.0	.0288323267	.0238565648	.0975695715
C	6.0	.0333727037	-.1384526451	2.9168183394
C	6.0	-.1490833192	-1.1964306623	.7602040829
C	6.0	.2251414032	1.1593626973	.8907205183
C	6.0	.2266466241	1.0785982054	2.2746426230
C	6.0	-.1538799246	-1.2769623131	2.1445207778
H	1.0	-.2767150465	-2.0982285980	.1871851601
H	1.0	.3806805703	2.0962348020	.3905100251
H	1.0	.3801811564	1.9726688401	2.8567398274
H	1.0	-.2955594770	-2.2337466534	2.6204128592
H	1.0	.0351282499	-.1997696363	3.9922356549
C	6.0	-.4036431586	-.7974317199	-2.2431067218
C	6.0	.4507372544	1.3391544094	-2.1363341495
H	1.0	-.8103609232	-1.7817878567	-2.1138827958

C	6.0	.2255799600	.9160545583	-3.3972983354
H	1.0	.3652292922	1.3717830490	-4.3582322020
O	8.0	-.2942099884	-.3766751848	-3.5020306164
Energy				-457.5622506807 Hartree
ZPE				.146515 HARTREE/MOLECULE
MP2/6-311+G(d,p)				-459.2484225596 Hartree
B3LYP/6-311+G(d,p)				-460.3052002960 Hartree

4'-carbanion of 3-phenylfuran

HF/6-31+G(d,p)

C	6.0	0.0158217274	0.1737512269	-1.2228674365
C	6.0	0.0148402356	-0.2817281743	0.1936669993
C	6.0	0.0003403249	-1.0386613434	2.8516954665
C	6.0	0.0360513585	-1.6791791649	0.4514400721
C	6.0	-0.0054731373	0.6845826111	1.2017289990
C	6.0	-0.0148094353	0.3145102430	2.5413116187
C	6.0	0.0279404425	-1.9844138781	1.8282739212
H	1.0	-0.0114187495	1.7370081068	0.9596334250
H	1.0	-0.0320941688	1.0641227562	3.3168749803
H	1.0	0.0423161803	-3.0253031996	2.1289297100
H	1.0	-0.0082237539	-1.3522584872	3.8865332817
C	6.0	0.1261014607	-0.5992970729	-2.3197146772
C	6.0	-0.1076831895	1.5214344534	-1.7514782230
H	1.0	0.2319467353	-1.6534655265	-2.4335048071
O	8.0	0.0827521734	0.1390952096	-3.4622942968
C	6.0	-0.0601390556	1.4182547103	-3.0881844452
H	1.0	-0.2224508473	2.4332610101	-1.2012936998
H	1.0	-0.1171978126	2.1414840327	-3.8746446081

Energy				-457.5497576335
ZPE				.146972 HARTREE/MOLECULE
MP2/6-311+G(d,p)				-459.2421124387 Hartree
B3LYP/6-311+G(d,p)				-460.2957340247 Hartree

NMR Spectra as Proof of Purity

N,N-dimethyl-4-(2-iodophenyl)aniline

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