***N,N*-Dimethyl- β -Alanine as an Inexpensive and Efficient Ligand for Palladium-Catalyzed Heck Reaction**

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Supporting Information

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(A) Typical Experimental Procedure

Typical experimental procedure for the ligands:

Synthesis of N,N-dimethyl- β -alanine hydrochloride¹: A mixture of 3.56g. of β -alanine, 25ml of 90% formic acid, 5.0ml of formalin was boiled under reflux for 8h, treated with 5ml of concentrated hydrochloride acid, evaporated to dryness, washed with acetic acid. The yield of colorless crystals, which melted at 189-191°C (uncorrected), was 2.1g.(35% of the calculated amount).

Synthesis of 4-(N,N-dimethylamino)butanoic acid hydrochloride²: N-methyl-2-pyrrolidinone 1.98g.(0.02mol), 12ml of water, and 3.2g of sodium hydroxide were heated at reflux for 10h. The solution was adjusted to pH 8 with 10% hydrochloride acid, evaporated to dryness. 6ml of 90% formic acid, 5ml of formalin was added, the solution was boiled under reflux for 8h, treated with 3ml of concentrated hydrochloride acid, evaporated to dryness, washed with acetic acid. The yield of colorless crystals, which melted at 148-150°C (uncorrected), was 2.4g.(73% of the calculated amount).

Typical experimental procedure for the Heck reaction: A mixture of aryl halide (1mmol), alkene (1.5mmol), Pd(OAc)₂ (10⁻³mmol), N,N-dimethyl- β -alanine hydrochloride (10⁻³mmol), K₂CO₃ (2mmol) in 1ml dry NMP was stirred under Ar at 130°C for the desired time. After the mixture was washed by water, extracted by ether and evaporated, the residue was purified by flash column chromatography (hexane/ethyl acetate) to afford the corresponding coupled products.

(B) Analytical Data

N,N-dimethyl- β -alanine hydrochloride³ (1) : ¹H NMR (300MHz, D₂O): δ 2.95 (m, 2H), 2.96 (s, 6H), 3.48 (t, 2H, J =6.51Hz); ¹³C NMR (75MHz, CDCl₃): δ 29.1, 43.2, 53.3, 174.1.

N,N-dimethylaminobutanoic acid hydrochloride⁴ (2) : ¹H NMR (300MHz, D₂O): δ 2.05 (m, 2H), 2.54 (t, 2H, J =6.75Hz), 2.93 (s, 6H), 3.22 (m, 2H); ¹³C NMR (75MHz, CDCl₃): δ 19.6, 30.6, 43.0, 57.0, 176.7.

Analytical data for the products of the Heck reaction:

trans-stilbene⁵: ¹H NMR (300MHz, CDCl₃): δ 7.11 (s, 2H), 7.23-7.27 (m, 2H), 7.36 (t, 4H, *J* = 7.5Hz), 7.51 (d, 4H, *J* = 7.7Hz); ¹³C NMR (75MHz, CDCl₃): δ 126.7, 127.8, 128.8, 128.9, 137.5.

trans-cinnamic acid *n*-butyl ester⁶: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* = 7.3Hz), 1.40-1.50 (m, 2H), 1.67-1.74 (m, 2H), 4.21 (t, 2H, *J* = 6.6Hz), 6.44 (d, 1H, *J* = 16.0Hz), 7.37-7.40 (m, 3H), 7.51-7.54 (m, 2H), 7.68 (d, 1H, *J* = 16.0Hz); ¹³C NMR (75MHz, CDCl₃): δ 13.7, 19.2, 30.8, 64.4, 118.3, 128.0, 128.8, 130.2, 134.5, 144.5, 167.0.

4-nitro-trans-stilbene⁵: ¹H NMR (300MHz, CDCl₃): δ 7.14 (d, 1H, *J* = 16.2Hz), 7.27 (d, 1H, *J* = 16.5Hz), 7.33-7.43 (m, 3H), 7.55 (d, 2H, *J* = 7.8Hz), 7.64 (d, 2H, *J* = 8.8Hz), 8.22 (d, 2H, *J* = 8.7Hz); ¹³C NMR (75MHz, CDCl₃): δ 124.3, 126.5, 127.0, 129.0, 129.1, 133.5, 136.4, 144.0, 147.0.

4-nitro-trans-cinnamic acid *n*-butyl ester⁷: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* = 7.4Hz), 1.38-1.51 (m, 2H), 1.66-1.75 (m, 2H), 4.24 (t, 2H, *J* = 6.7Hz), 6.56 (d, 1H, *J* = 16.1Hz), 7.67 (d, 2H, *J* = 8.7Hz), 7.70 (d, 1H, *J* = 15.7Hz), 8.25 (d, 2H, *J* = 8.7Hz); ¹³C NMR (75MHz, CDCl₃): δ 13.9, 19.3, 30.9, 65.1, 122.8, 124.3, 128.8, 140.8, 141.7, 148.7, 166.3.

4-methyl-trans-stilbene⁵: ¹H NMR (300MHz, CDCl₃): δ 2.36 (s, 3H), 7.07 (s, 2H), 7.17 (d, 2H, *J* = 8.0Hz), 7.24-7.26 (m, 1H), 7.35 (t, 2H, *J* = 7.5Hz), 7.41 (d, 2H, *J* = 8.1Hz), 7.51 (d, 2H, *J* = 7.9Hz); ¹³C NMR (75MHz, CDCl₃): δ 21.4, 126.5, 126.6, 127.5, 127.9, 128.8, 129.5, 134.7, 137.7.

(8)

4-methyl-*trans*-cinnamic acid *n*-butyl ester⁶: ¹H NMR (300MHz, CDCl₃): δ 0.96 (t, 3H, *J* = 7.4Hz), 1.40-1.47 (m, 2H), 1.64-1.73 (m, 2H), 4.20 (t, 2H, *J* = 6.7Hz), 6.34 (d, 1H, *J* = 16.0Hz), 7.18 (d, 2H, *J* = 8.0Hz), 7.42 (d, 2H, *J* = 8.0Hz), 7.65 (d, 1H, *J* = 16.0Hz), ¹³C NMR (75MHz, CDCl₃): δ 13.8, 19.3, 21.5, 30.8, 64.4, 117.3, 128.1, 129.7, 131.9, 140.7, 144.6, 167.3.

(9)

***trans*-3-naphthalen-1-yl-acrylic acid *n*-butyl ester⁸:** ¹H NMR (300MHz, CDCl₃): δ 0.98 (t, 3H, *J* = 7.3Hz), 1.40-1.53 (m, 2H), 1.68-1.77 (m, 2H), 4.26 (t, 2H, *J* = 6.7Hz), 6.52 (d, 1H, *J* = 15.8Hz), 7.45-7.55 (m, 3H), 7.73 (d, 1H, *J* = 7.2Hz), 7.84-7.87 (m, 2H), 8.18 (d, 1H, *J* = 8.2Hz), 8.52 (d, 1H, *J* = 15.8Hz); ¹³C NMR (75MHz, CDCl₃): δ 13.8, 19.3, 30.9, 64.5, 121.0, 123.4, 125.0, 125.4, 126.2, 126.8, 128.7, 130.4, 131.4, 131.8, 133.7, 141.5, 166.9.

(10)

4-methoxy-*trans*-stilbene⁶: ¹H NMR (300MHz, CDCl₃): δ 3.83 (s, 3H), 6.90 (d, 2H, *J* = 8.7Hz), 6.98 (d, 1H, *J* = 16.4Hz), 7.08 (d, 1H, *J* = 16.3Hz), 7.23 (t, 1H, *J* = 7.0Hz), 7.34 (t, 2H, *J* = 7.5Hz), 7.44-7.50 (m, 4H); ¹³C NMR (75MHz, CDCl₃): δ 55.5, 114.3, 126.4, 126.8, 127.3, 127.9, 128.4, 128.8, 130.3, 137.8, 159.5.

(11)

4-methoxy-*trans*-cinnamic acid *n*-butyl ester⁶: ¹H NMR (300MHz, CDCl₃): δ 0.96 (t, 3H, *J* = 7.4Hz), 1.40-1.47 (m, 2H), 1.64-1.71 (m, 2H), 3.83 (s, 3H), 4.20 (t, 2H, *J* = 6.7Hz), 6.31 (d, 1H, *J* = 15.9Hz), 6.90 (d, 2H, *J* = 8.7Hz), 7.47 (d, 2H, *J* = 8.7Hz), 7.63 (d, 1H, *J* = 16.0Hz), ¹³C NMR (75MHz, CDCl₃): δ 13.8, 19.3, 30.9, 55.3, 64.3, 114.4, 115.8, 127.3, 129.7, 144.2, 161.4, 167.4.

(12)

***trans*-stilbene-4-carboxylic acid⁹:** ¹H NMR (300MHz, acetone-d₆): δ 7.31-7.43 (5H), 7.66 (d, 2H, *J* = 7.8Hz), 7.74 (d, 2H, *J* = 8.5Hz), 8.04 (d, 2H, *J* = 8.4Hz), 11.10 (s, 1H); ¹³C NMR (75MHz, acetone-d₆): δ 127.3, 127.7, 128.4, 129.0, 129.6, 130.2, 131.0, 132.1, 138.0, 143.0, 167.3,.

4-formyl-*trans*-stilbene⁶: ¹H NMR (300MHz, CDCl₃): δ 7.12 (d, 1H, *J* =16.4Hz), 7.24 (d, 1H, *J* =16.4Hz), 7.27-7.35 (m, 1H), 7.39 (t, 2H, *J* =5.1Hz), 7.51-7.54 (m, 2H), 7.63 (d, 2H, *J* =8.2Hz), 7.85 (d, 2H, *J* =8.2Hz), 9.98 (s, 1H); ¹³C NMR (75MHz, CDCl₃): δ 127.0, 127.4, 128.6, 128.9, 130.3, 132.3, 135.4, 136.6, 143.5, 191.6.

4-formyl-*trans*-cinnamic acid *n*-butyl ester⁶: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* =7.4Hz), 1.41-1.48 (m, 2H), 1.64-1.73 (m, 2H), 4.23 (t, 2H, *J* =6.7Hz), 6.56 (d, 1H, *J* =16.1Hz), 7.68 (d, 2H, *J* =8.2Hz), 7.71 (d, 1H, *J* =16.1Hz), 7.90 (d, 2H, *J* =8.2Hz), 10.03 (s, 1H); ¹³C NMR (75MHz, CDCl₃): δ 13.8, 19.2, 30.8, 64.8, 121.6, 128.5, 130.2, 137.2, 140.2, 142.8, 166.4, 191.4.

4-acetyl-*trans*-stilbene¹⁰: ¹H NMR (300MHz, CDCl₃): δ 2.61 (s, 3H), 7.14 (d, 1H, *J* =16.4Hz), 7.22 (d, 1H, *J* =16.4Hz), 7.25-7.38 (m, 3H), 7.55 (d, 2H, *J* =7.9Hz), 7.59 (d, 2H, *J* =8.4Hz), 7.95 (d, 2H, *J* =8.4Hz); ¹³C NMR (75MHz, CDCl₃): δ 26.7, 126.6, 126.9, 127.6, 128.4, 128.9, 129.0, 131.6, 136.1, 136.8, 142.1, 197.6.

4-acetyl-*trans*-cinnamic acid *n*-butyl ester¹¹: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* =7.3Hz), 1.41-1.48 (m, 2H), 1.65-1.73 (m, 2H), 2.61 (s, 3H), 4.23 (t, 2H, *J* =6.6Hz), 6.53 (d, 1H, *J* =16.0Hz), 7.61 (d, 2H, *J* =8.3Hz), 7.69 (d, 1H, *J* =16.1Hz), 7.97 (d, 2H, *J* =8.3Hz); ¹³C NMR (75MHz, CDCl₃): δ 13.7, 19.2, 26.6, 30.7, 64.6, 120.8, 128.1, 128.8, 138.0, 138.8, 142.9, 166.5, 197.1.

***trans*-stilben-4-ol¹²:** ¹H NMR (300MHz, acetone-d₆): δ 6.85 (d, 2H, *J* =7.7Hz), 7.05 (d, 1H, *J* =16.4Hz), 7.16 (d, 1H, *J* =16.4Hz), 7.19-7.21 (m, 1H), 7.34 (t, 2H, *J* =7.6Hz), 7.45 (d, 2H, *J* =7.8Hz), 7.55 (d, 2H, *J* =7.9Hz), 8.44 (s, 1H); ¹³C NMR (75MHz, acetone-d₆): δ 116.5, 126.5, 127.0, 127.8, 128.8, 129.4, 129.5, 130.0, 138.9, 158.3.

(18)

***trans*-3-(4-hydroxy-phenyl)-acrylic acid *n*-butyl ester**¹³: ¹H NMR (300MHz, CDCl₃): δ 0.96 (t, 3H, *J* = 7.3Hz), 1.40-1.50 (m, 2H), 1.64-1.74 (m, 2H), 4.21 (t, 2H, *J* = 6.6Hz), 5.95 (s, 1H), 6.30 (d, 1H, *J* = 15.9Hz), 6.86 (d, 2H, *J* = 8.6Hz), 7.42 (d, 2H, *J* = 8.6Hz), 7.62 (d, 1H, *J* = 15.9Hz); ¹³C NMR (75MHz, CDCl₃): δ 13.8, 19.3, 30.8, 64.9, 115.1, 116.1, 126.8, 130.2, 145.3, 158.6, 168.6.

(19)

***trans*-stilbene-3-carbonitrile**¹⁴: ¹H NMR (300MHz, CDCl₃): δ 7.06 (d, 1H, *J* = 16.4Hz), 7.14 (d, 1H, *J* = 16.4Hz), 7.30-7.54 (m, 7H), 7.70 (m, 1H), 7.77 (s, 1H); ¹³C NMR (75MHz, CDCl₃): δ 113.0, 118.8, 126.2, 126.8, 128.5, 128.9, 129.5, 129.9, 130.6, 130.7, 131.4, 136.4, 138.6.

(20)

***trans*-3-(3-cyano-phenyl)-acrylic acid *n*-butyl ester**: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* = 7.4Hz), 1.40-1.48 (m, 2H), 1.66-1.75 (m, 2H), 4.23 (t, 2H, *J* = 6.6Hz), 6.49 (d, 1H, *J* = 16.0Hz), 7.51 (t, 1H, *J* = 7.8Hz), 7.61-7.66 (m, 2H), 7.73-7.76 (m, 1H), 7.80 (s, 1H); ¹³C NMR (75MHz, CDCl₃): δ 13.8, 19.2, 30.8, 64.8, 113.4, 118.2, 121.2, 129.9, 131.4, 131.9, 133.2, 135.8, 141.8, 166.3; HRMS (EI): 229.1111(M⁺).

(21)

***trans*-stilbene-4-carbonitrile**⁶: ¹H NMR (300MHz, CDCl₃): δ 7.08 (d, 1H, *J* = 16.4Hz), 7.20 (d, 1H, *J* = 16.3Hz), 7.31-7.40 (m, 3H), 7.51-7.64 (m, 6H); ¹³C NMR (75MHz, CDCl₃): δ 110.6, 119.1, 126.8, 126.9, 127.0, 128.7, 128.9, 132.5, 132.5, 136.4, 141.9.

(22)

***trans*-3-(4-cyano-phenyl)-acrylic acid *n*-butyl ester**⁶: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* = 7.4Hz), 1.38-1.50 (m, 2H), 1.65-1.74 (m, 2H), 4.23 (t, 2H, *J* = 6.6Hz), 6.53 (d, 1H, *J* = 16.1Hz), 7.60-7.70 (m, 5H); ¹³C NMR (75MHz, CDCl₃): δ 13.6, 19.1, 30.6, 64.7, 113.2, 118.2, 121.8, 128.3, 132.5, 138.7, 142.0, 166.1.

4-phenyl-*trans*-stilbene: ^1H NMR (300MHz, CDCl_3): δ 7.15 (s, 2H), 7.25 (m, 1H), 7.34-7.45 (m, 5H), 7.52-7.64 (m, 8H); ^{13}C NMR (75MHz, CDCl_3): δ 126.7, 127.1, 127.1, 127.5, 127.5, 127.8, 128.4, 128.9, 128.9, 128.9, 136.6, 137.5, 140.5, 140.8; HRMS (EI): 256.1247(M^+).

4-phenyl-*trans*-cinnamic acid *n*-butyl ester: ^1H NMR (300MHz, CDCl_3): δ 0.97 (t, 3H, $J=7.3\text{Hz}$), 1.39-1.51 (m, 2H), 1.66-1.75 (m, 2H), 4.22 (t, 2H, $J=6.6\text{Hz}$), 6.47 (d, 1H, $J=16.0\text{Hz}$), 7.30-7.39 (m, 1H), 7.42-7.47 (m, 2H), 7.59-7.62 (m, 6H), 7.72 (d, 1H, $J=16.0\text{Hz}$); ^{13}C NMR (75MHz, CDCl_3): δ 13.8, 19.3, 30.9, 64.5, 118.2, 127.1, 127.6, 127.9, 128.6, 129.0, 133.5, 140.2, 143.0, 144.1, 167.2; HRMS (EI): 280.1456(M^+).

3-trifluoromethyl-*trans*-stilbene¹⁵: ^1H NMR (300MHz, CDCl_3): δ 7.11 (d, 1H, $J=16.4\text{Hz}$), 7.17 (d, 1H, $J=16.4\text{Hz}$), 7.29 (m, 1H), 7.35-7.40 (m, 2H), 7.46-7.54 (m, 4H), 7.66 (m, 1H), 7.76 (s, 1H); ^{13}C NMR (75MHz, CDCl_3): δ 123.2 (q, $J=3.8\text{Hz}$), 124.2 (q, $J=3.8\text{Hz}$), 124.3 (q, $J=271\text{Hz}$), 126.9, 127.3, 128.3, 128.9, 129.2, 129.7, 130.7, 131.3 (q, $J=32.0\text{Hz}$), 136.8, 138.3.

3- trifluoromethyl-*trans*-cinnamic acid *n*-butyl ester: ^1H NMR (300MHz, CDCl_3): δ 0.97 (t, 3H, $J=7.3\text{Hz}$), 1.38-1.51 (m, 2H), 1.65-1.75 (m, 2H), 4.23 (t, 2H, $J=6.6\text{Hz}$), 6.51 (d, 1H, $J=16.1\text{Hz}$), 7.51 (t, 1H, $J=7.7\text{Hz}$), 7.62 (d, 1H, $J=7.7\text{Hz}$), 7.69 (d, 1H, $J=16.0\text{Hz}$), 7.70 (d, 1H, $J=8.0\text{Hz}$), 7.77 (s, 1H); ^{13}C NMR (75MHz, CDCl_3): δ 13.7, 19.2, 30.8, 64.7, 120.4, 123.9 (q, $J=271\text{Hz}$), 124.6 (q, $J=3.8\text{Hz}$), 126.6 (q, $J=3.7\text{Hz}$), 129.5, 131.1, 131.5 (q, $J=32.3\text{Hz}$), 135.4, 142.7, 166.5; HRMS (EI): 272.1023(M^+).

3-*trans*-styryl-pyridine¹⁶: ^1H NMR (300MHz, CDCl_3): δ 7.06 (d, 1H, $J=16.4\text{Hz}$), 7.16 (d, 1H, $J=16.3\text{Hz}$), 7.26-7.40 (m, 4H), 7.53 (m, 2H), 7.85 (d, 1H, $J=9.0\text{Hz}$), 8.48 (m, 1H), 8.72 (s, 1H); ^{13}C NMR (75MHz, CDCl_3): δ 123.5, 124.9, 126.7, 128.2, 128.4, 128.8, 130.8, 132.6, 133.0, 136.7, 148.6.

3-pyridin-3-yl-acrylic acid butyl ester⁶: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 3H, *J* = 7.4Hz), 1.38-1.50 (m, 2H), 1.65-1.75 (m, 2H), 4.23 (t, 2H, *J* = 6.6Hz), 6.52 (d, 1H, *J* = 16.1Hz), 7.31-7.35 (m, 1H), 7.67 (d, 1H, *J* = 16.1Hz); 7.84 (d, 1H, *J* = 7.8Hz), 8.60 (m, 1H), 8.75 (s, 1H); ¹³C NMR (75MHz, CDCl₃): δ 13.6, 19.1, 30.6, 64.5, 120.4, 123.6, 130.1, 134.1, 140.7, 149.6, 150.8, 166.2.

1,4-di(2-n-butylcarbonyl-*trans*-vinyl)-benzene¹⁷: ¹H NMR (300MHz, CDCl₃): δ 0.97 (t, 6H, *J* = 7.3Hz), 1.40-1.48 (m, 4H), 1.61-1.72 (m, 4H), 4.22 (t, 4H, *J* = 6.6Hz), 6.47 (d, 2H, *J* = 16.0Hz), 7.54 (s, 4H), 7.66 (d, 2H, *J* = 16.0Hz); ¹³C NMR (75MHz, CDCl₃): δ 13.7, 19.2, 30.8, 64.5, 119.4, 128.5, 136.2, 143.4, 166.8.

(C) References

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(D) Spectra

N,N-dimethyl- β -alanine hydrochloride (1)

N,N-dimethyl- β -alanine hydrochloride (1)

N,N-dimethylaminobutanoic acid hydrochloride (2)

N,N-dimethylaminobutanoic acid hydrochloride (2)

trans-stilbene (3)

trans-stilbene (3)

trans-cinnamic acid *n*-butyl ester (4)

***trans*-cinnamic acid *n*-butyl ester (4)**

4-nitro-*trans*-stilbene (5)

4-nitro-*trans*-stilbene (5)

4-nitro-*trans*-cinnamic acid *n*-butyl ester (6)

4-nitro-*trans*-cinnamic acid *n*-butyl ester (6)

4-methyl-*trans*-stilbene (7)

4-methyl-*trans*-stilbene (7)

4-methyl-*trans*-cinnamic acid *n*-butyl ester (8)

4-methyl-*trans*-cinnamic acid *n*-butyl ester (8)

***trans*-3-naphthalen-1-yl-acrylic acid *n*-butyl ester (9)**

***trans*-3-naphthalen-1-yl-acrylic acid *n*-butyl ester (9)**

4-methoxy-*trans*-stilbene (10)

4-methoxy-*trans*-stilbene (10)

4-methoxy-*trans*-cinnamic acid *n*-butyl ester (11)

4-methoxy-*trans*-cinnamic acid *n*-butyl ester (11)

***trans*-stilbene-4-carboxylic acid (12)**

***trans*-stilbene-4-carboxylic acid (12)**

4-formyl-*trans*-stilbene (13)

4-formyl-*trans*-stilbene (13)

4-formyl-*trans*-cinnamic acid *n*-butyl ester (14)

4-formyl-*trans*-cinnamic acid *n*-butyl ester (14)

4-acetyl-*trans*-stilbene (15)

4-acetyl-*trans*-stilbene (15)

4-acetyl-*trans*-cinnamic acid *n*-butyl ester (16)

4-acetyl-*trans*-cinnamic acid *n*-butyl ester (16)

***trans*-stilben-4-ol (17)**

trans-stilben-4-ol (17)

***trans*-3-(4-hydroxy-phenyl)-acrylic acid *n*-butyl ester (18)**

***trans*-3-(4-hydroxy-phenyl)-acrylic acid *n*-butyl ester (18)**

trans-stilbene-3-carbonitrile (19)

***trans*-stilbene-3-carbonitrile (19)**

***trans*-3-(3-cyano-phenyl)-acrylic acid *n*-butyl ester (20)**

***trans*-3-(3-cyano-phenyl)-acrylic acid *n*-butyl ester (20)**

trans-stilbene-4-carbonitrile (21)

trans-stilbene-4-carbonitrile (21)

***trans*-3-(4-cyano-phenyl)-acrylic acid *n*-butyl ester (22)**

***trans*-3-(4-cyano-phenyl)-acrylic acid *n*-butyl ester (22)**

4-phenyl-*trans*-stilbene (23)

4-phenyl-*trans*-stilbene (23)

4-phenyl-*trans*-cinnamic acid *n*-butyl ester (24)

4-phenyl-*trans*-cinnamic acid *n*-butyl ester (24)

3-trifluormethyl-*trans*-stilbene (25)

3-trifluormethyl-*trans*-stilbene (25)

3- trifluormethyl-*trans*-cinnamic acid *n*-butyl ester (26)

3- trifluormethyl-*trans*-cinnamic acid *n*-butyl ester (26)

3-*trans*-styryl-pyridine (27)

3-trans-styryl-pyridine (27)

3-pyridin-3-yl-acrylic acid butyl ester (28)

3-pyridin-3-yl-acrylic acid butyl ester (28)

1,4-di(2-n-butylcarbonyl-*trans*-vinyl)-benzene (29)

1,4-di(2-n-butylcarbonyl-*trans*-vinyl)-benzene (29)

(E) Computational Data

Pd(L1)(η^2 -PhBr)

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -733.8610488

Tcg (Hartree) = 0.146895

DeltaG (solv kcal/mol) = -40.83

Charge = -1 Multiplicity = 1

Pd	0.36007800	0.44581400	-0.20653700
N	1.88600000	-0.85036100	0.88177600
C	1.37311700	-2.20287300	1.18670600
O	2.31748300	1.28961800	-0.80702700
C	3.34253100	0.48961700	-0.69489700
O	4.53267500	0.69980700	-1.07983200
C	3.04541600	-0.89270800	-0.04944300
C	2.23940100	-0.12082200	2.12292200
H	0.50694800	-2.12087900	1.85038800
H	1.03745500	-2.68148600	0.26314400
H	2.14350800	-2.83458000	1.67120700
H	1.35145500	-0.02975200	2.75623300
H	3.03761200	-0.64485500	2.68451400
H	2.58291000	0.88245000	1.85932100
H	2.80442600	-1.58987300	-0.86202500
H	3.95843500	-1.25314000	0.45457600
C	-1.60497000	0.10742600	0.04315800
C	-1.53391600	1.13744900	-0.99712000
H	-1.45867700	0.84963100	-2.04389100
C	-2.19376500	0.43951900	1.31950800
C	-2.61678700	1.73598700	1.57504000
H	-2.29341400	-0.33816700	2.07277900
H	-3.01158400	1.98262700	2.55997600
C	-2.02383900	2.45118400	-0.68258100
C	-2.53813000	2.75235000	0.57136800
H	-2.00586900	3.21071000	-1.46340500
H	-2.89326900	3.75684800	0.79294800
Br	-2.15031900	-1.85836000	-0.58687400

[Pd(L1)(PhBr)][±]

Number of Imaginary Frequency = 1

Electronic Energy (Hartree) = -733.845211436

Tcg (Hartree) = 0.149296

DeltaG (solv kcal/mol) = -44.6

Charge = -1 Multiplicity = 1

Pd	0.28071000	-0.13890300	-0.26622300
C	-1.62965600	-0.21531200	0.15879100
Br	-1.77228300	2.13286700	0.07015600
C	-1.97734700	-0.77982100	-1.11103800
H	-1.78618600	-0.22241000	-2.02458400
O	1.51924700	0.18552400	1.63104200
N	2.43253500	-0.18819500	-0.96346500
C	-2.12756300	-0.79006800	1.36292400
C	-2.72906100	-1.98153500	-1.14466300
C	2.72145400	-0.31109800	1.55967300
C	3.16410600	-0.83368800	0.16227700
C	2.83827500	1.23425300	-1.09912400
C	2.63720400	-0.92045500	-2.23218400
C	-3.17940500	-2.57061000	0.04239200
C	-2.88013800	-1.96348200	1.29167900
O	3.56340100	-0.44878200	2.50022900
H	-2.99133000	-2.41999000	-2.10712900
H	-3.77234400	-3.48271600	0.01145200
H	-3.22141900	-2.43317000	2.21318400
H	-1.87053900	-0.33378000	2.31330500
H	2.94984700	-1.90985700	0.13462400
H	4.25450000	-0.69588800	0.06494400
H	3.91347200	1.32351000	-1.34606100
H	2.24513600	1.71106600	-1.88616100
H	2.63727700	1.74692400	-0.15569800
H	3.70400200	-0.94478800	-2.52841400
H	2.27731900	-1.94773700	-2.11964600
H	2.06136400	-0.43763700	-3.02931000

PhPd(L1)Br

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -733.922862838

Tcg (Hartree) = 0.151421

DeltaG (solv kcal/mol) = -40.97

Charge = -1 Multiplicity = 1

C	4.53017100	1.13277200	0.02956700
C	3.56621300	1.98074200	-0.54457900
C	2.20588700	1.62061200	-0.53993000
C	1.77931500	0.39565800	0.02457700
C	2.75547300	-0.44832100	0.60135500
C	4.11498700	-0.07949100	0.60799600
Pd	-0.17707600	0.00622700	0.00302800
O	-0.63189500	2.03667000	0.20731900
C	-1.87976300	2.39300700	-0.03034300
C	-2.82716400	1.25523300	-0.46722800

N	-2.42096000	-0.07367000	0.06923900
C	-2.74904200	-0.18775600	1.51428600
Br	0.13277800	-2.51820700	-0.19607900
C	-3.05300900	-1.17429700	-0.69707800
O	-2.33373100	3.56747200	0.02427000
H	1.46482100	2.30508100	-0.94254300
H	3.86859100	2.93012400	-0.98621600
H	5.58282200	1.41297700	0.02970300
H	4.84854100	-0.74740500	1.05960600
H	2.45555600	-1.40032500	1.02843100
H	-3.84164100	-0.14414400	1.67884000
H	-2.35894200	-1.13683600	1.89244100
H	-2.26874400	0.62896400	2.05995000
H	-4.15552100	-1.12473400	-0.62789000
H	-2.74934500	-1.10603100	-1.74542200
H	-2.69276300	-2.13180400	-0.31275900
H	-2.78393100	1.20519900	-1.56253100
H	-3.85787100	1.51332300	-0.17725900

Pd(L2)(η^2 -PhBr)

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -773.14421446

Tcg (Hartree) = 0.174375

DeltaG (solv kcal/mol) = -42.24

Charge = -1 Multiplicity = 1

Pd	0.30329800	0.43596600	-0.10257100
N	1.45490600	-1.29201200	0.80291800
C	0.67335600	-1.76812300	1.97004400
O	2.19855400	1.41831100	-0.53039600
C	1.55313800	-2.37383700	-0.20620400
H	2.12493900	-3.23962800	0.18332100
H	0.54126400	-2.69296600	-0.47220000
H	2.03717400	-2.00149900	-1.11089900
H	1.17351700	-2.62351700	2.46765400
H	0.56097300	-0.95142800	2.68920600
H	-0.32098500	-2.07481400	1.63439600
C	3.41849700	0.96351900	-0.58974400
C	2.78929600	-0.80514700	1.26763500
H	2.59301900	0.02809200	1.95310700
H	3.27177200	-1.61925800	1.85017800
C	3.76036900	-0.34073900	0.18040800
H	4.73669600	-0.16561000	0.65185500
H	3.93645200	-1.12881500	-0.56450500
O	4.38239300	1.49252900	-1.22839400
C	-1.68164400	0.24092500	0.03112400

C	-1.52965700	1.36544400	-0.89065500
H	-1.37648800	1.18287800	-1.95213200
C	-1.98370700	2.65849300	-0.47352700
C	-2.55158700	2.85565700	0.77983200
H	-1.89344500	3.49001600	-1.17128400
H	-2.88026500	3.84690000	1.08548700
C	-2.32087500	0.46812300	1.30464600
C	-2.71459500	1.74933600	1.66824900
H	-2.48127400	-0.37314800	1.97410300
H	-3.14902700	1.91154200	2.65421300
Br	-2.34667100	-1.65622100	-0.82729200

[Pd(L2)(PhBr)][‡]

Number of Imaginary Frequency = 1

Electronic Energy (Hartree) = -773.131703245

Tcg (Hartree) = 0.175395

DeltaG (solv kcal/mol) = -44.17

Charge = -1 Multiplicity = 1

C	1.70839600	-0.01711300	0.17611700
Br	1.54206900	-1.87869500	-1.23186700
C	2.14184600	1.12284500	-0.57901300
H	1.89311800	1.20127400	-1.63418800
C	2.26899400	-0.28779400	1.45803000
C	3.06002400	2.02850000	0.01242900
C	3.57694400	1.78332000	1.28920500
C	3.17928100	0.61874100	2.00191700
H	3.39483700	2.89598900	-0.55624800
H	4.29435100	2.47148400	1.73257100
H	3.56995100	0.44238600	3.00335800
H	1.92988100	-1.15984100	2.00694600
Pd	-0.19007700	0.41810100	-0.04794900
N	-2.20932600	1.31093600	-0.59910100
O	-1.14345500	-0.87303900	1.51411200
C	-2.19053200	2.75172400	-0.24829400
C	-2.37389700	1.14514100	-2.06403000
C	-3.30399900	0.61537700	0.14839700
C	-2.33294900	-1.40618200	1.39724100
H	-3.15383700	3.24516500	-0.48676600
H	-1.98775900	2.85694400	0.82093500
H	-1.38752500	3.25031300	-0.80012400
H	-3.32969500	1.58131100	-2.41629600
H	-1.54324700	1.63607700	-2.58036300
H	-2.35181500	0.08409000	-2.32259300
H	-3.28677100	1.00114700	1.17400600
H	-4.27444100	0.90883200	-0.30112500

C	-3.17885100	-0.91804000	0.19469400
O	-2.85262900	-2.25556200	2.18646300
H	-4.17572500	-1.36547100	0.27826900
H	-2.71781100	-1.29487700	-0.72843700

PhPd(L2)Br

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -773.211769439

Tcg (Hartree) = 0.179852

DeltaG (solv kcal/mol) = -39.81

Charge = -1 Multiplicity = 1

C	-4.57623100	1.00879700	-0.04832400
C	-3.69686700	1.68867200	0.81373400
C	-2.32724800	1.36689700	0.83547500
C	-1.81160400	0.34413700	0.00899000
C	-2.70058400	-0.33391600	-0.85423100
C	-4.06850900	0.00137800	-0.88712100
Br	-0.27008700	-2.57635400	0.02505100
H	-1.64401100	1.93700100	1.45773200
H	-4.07205100	2.48215200	1.45977900
H	-5.63545500	1.26239100	-0.06896300
H	-4.73558400	-0.53448400	-1.56238000
H	-2.33023800	-1.13727000	-1.48408100
Pd	0.14543400	-0.04174600	0.07741600
N	2.39870500	-0.37259700	0.12366500
O	0.42357600	2.00843000	0.32401800
C	2.71827400	-1.11050600	1.37535200
C	2.78989200	-1.19205000	-1.05414500
C	3.12047000	0.93684400	0.10781400
C	1.37043600	2.73745100	-0.23877600
H	3.80693400	-1.28489800	1.46910100
H	2.36898700	-0.52933600	2.23399800
H	2.18671900	-2.06566700	1.36589900
H	3.87142100	-1.42412400	-1.02814900
H	2.20542400	-2.11558800	-1.05042900
H	2.56471700	-0.64977500	-1.97657300
H	3.07449200	1.35092600	1.12141300
H	4.18605400	0.74922900	-0.12417200
C	2.53322700	1.96104100	-0.87635700
O	1.39388000	3.99990200	-0.23100700
H	3.30098900	2.68428200	-1.17121400
H	2.17656300	1.45691600	-1.78410100

Pd(L3)(η^2 -PhBr)

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -812.441048756

Tcg (Hartree) = 0.203392

DeltaG (solv kcal/mol) = -36.84

Charge = -1 Multiplicity = 1

C	-1.81290900	0.11428900	-0.05247300
C	-1.60137600	1.28783300	-0.90691800
H	-1.39287500	1.16002700	-1.96709100
C	-2.12306100	2.55003300	-0.46046500
C	-2.80454400	2.66870100	0.74347700
H	-1.99028700	3.41972800	-1.10252800
H	-3.17891800	3.63721800	1.06898200
C	-2.58413000	0.25978900	1.16035800
C	-3.03266400	1.51252800	1.55412000
H	-2.80190300	-0.62274100	1.75745500
H	-3.56586200	1.61475400	2.49865400
Br	-2.27261600	-1.71295800	-1.05558800
Pd	0.17446500	0.48377200	0.01815800
N	1.36467800	-1.06357500	1.28582800
O	2.01553400	1.66397100	-0.27267400
C	0.95626200	-0.71778800	2.67011100
C	0.92129100	-2.43453600	0.94974300
C	2.84503400	-0.90847800	1.16993100
C	3.04383900	1.18544100	-0.93384600
H	1.42244200	-1.39868800	3.41152000
H	1.26029000	0.31008200	2.88752700
H	-0.13187800	-0.77883300	2.75632000
H	1.42184100	-3.19030900	1.58865000
H	-0.16173600	-2.50503400	1.07893400
H	1.13462800	-2.65192500	-0.09859100
C	3.45105700	-1.20217100	-0.21062400
H	3.07312200	0.12727200	1.44234900
H	3.32735400	-1.57495100	1.91613600
C	2.93700500	-0.29740300	-1.35164900
O	4.12038200	1.81165700	-1.19076700
H	4.53528300	-1.04843500	-0.10921000
H	3.30801800	-2.26037800	-0.47553800
H	3.55151900	-0.46853000	-2.24413300
H	1.89022400	-0.53867600	-1.58297400

[Pd(L3)(PhBr)][‡]

Number of Imaginary Frequency = 1

Electronic Energy (Hartree) = -812.429964105

Tcg (Hartree) = 0.203292

DeltaG (solv kcal/mol) = -37.12

Charge = -1 Multiplicity = 1

Pd	-0.09682700	-0.45059800	-0.39949800
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N	-1.21909500	-0.23331200	1.73757700
O	-1.89831200	-1.26451200	-1.31311400
C	-0.63022700	-1.34788000	2.51536500
C	-0.92811000	1.06066600	2.38474900
C	-2.68266800	-0.47248100	1.58026700
C	-3.02545400	-0.59278700	-1.39283000
H	-1.04348200	-1.39008400	3.54497700
H	-0.84573900	-2.29322400	2.00868400
H	0.45547000	-1.22851400	2.56678500
H	-1.41806600	1.14141100	3.37721400
H	0.15282800	1.16631900	2.51022800
H	-1.26007500	1.88404300	1.74991500
C	-3.46908300	0.59014800	0.79704900
H	-2.78969600	-1.43642500	1.07148200
H	-3.13606800	-0.56577000	2.59123400
C	-3.04138400	0.77271100	-0.67551700
O	-4.09303300	-1.00394900	-1.94569400
H	-4.52013400	0.26653300	0.81235000
H	-3.43201400	1.55711400	1.32059000
H	-3.76453300	1.43020700	-1.17362800
H	-2.04605300	1.23277600	-0.72811100
Br	1.27155700	2.17328000	-0.46569500
C	1.86499600	0.05270800	-0.08258200
C	2.25602700	-0.64107500	-1.27567900
C	2.61425900	-0.14636500	1.11529900
C	3.29071900	-1.60041500	-1.21646200
H	1.81700600	-0.36078300	-2.23090700
C	3.64917700	-1.08565300	1.13756400
H	2.37400900	0.43182200	2.00394800
C	3.98766900	-1.82927100	-0.02068900
H	3.56313900	-2.14363100	-2.12032900
H	4.19532300	-1.25394500	2.06545600
H	4.79653200	-2.55609900	0.01458700

PhPd(L3)Br

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -812.504745853

Tcg (Hartree) = 0.207725

DeltaG (solv kcal/mol) = -36.19

Charge = -1 Multiplicity = 1

N	-2.30385600	-0.62714400	-0.29773700
C	-2.41609300	-1.34550200	-1.59767400
O	-0.45513200	1.86181200	-0.61802600
C	-2.72217300	-1.52328600	0.80990200
H	-3.79612400	-1.77847200	0.72872000

H	-2.11592300	-2.43184600	0.77478300
H	-2.53930600	-1.03851600	1.77206000
H	-3.46095300	-1.65628300	-1.79142400
H	-2.08392800	-0.68268400	-2.40258800
H	-1.76469100	-2.22316800	-1.57696700
C	-1.15259600	2.67153600	0.16482600
C	-3.20641800	1.44986300	0.92163300
H	-3.87637100	2.29437800	0.70511900
H	-3.66627900	0.88789900	1.74677400
C	-1.83942000	2.01441400	1.36868900
H	-1.99727100	2.76710800	2.14953300
H	-1.20357900	1.21206100	1.76263300
O	-1.34541100	3.89608300	-0.08018100
C	-3.16572500	0.59411400	-0.35399300
H	-2.79903500	1.20364700	-1.18645700
H	-4.20069100	0.27753700	-0.59456700
Pd	-0.05118900	-0.13304900	-0.15974700
C	1.87009300	0.38284600	-0.04344400
C	2.37429000	1.32840500	-0.96371000
C	2.74300600	-0.12428400	0.94472800
C	3.71845300	1.74128400	-0.90864500
H	1.69961200	1.76847400	-1.69234900
C	4.08360000	0.30321900	1.00889700
H	2.38352100	-0.86843400	1.64946400
C	4.58141600	1.23245800	0.07871100
H	4.08516000	2.47216300	-1.62906300
H	4.73849800	-0.10041000	1.78106500
H	5.62018700	1.55701000	0.12478700
Br	0.53293200	-2.61610800	0.11763200

Pd(OAc)₂(η²-PhBr)

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -828.296357058

Tcg (Hartree) = 0.115263

DeltaG (solv kcal/mol) = -151.52

Charge = -2 Multiplicity = 1

Pd	-0.32620800	-0.24382600	-0.01832600
C	1.65959300	-0.13695300	0.12991700
C	1.42232000	-1.52018300	-0.30036600
H	1.33670300	-1.75081700	-1.36070900
C	2.24408200	0.09429800	1.43022900
C	2.50852100	-0.97291500	2.27942500
H	2.43972200	1.11850600	1.73690200
H	2.88166600	-0.77301600	3.28488700
C	1.74777100	-2.58219300	0.60802100

C	2.26714600	-2.32396200	1.87241600
H	1.59041000	-3.61104000	0.28148000
H	2.48377500	-3.14303700	2.55790900
Br	2.63400100	1.14176500	-1.37370400
O	-4.17914300	-2.05319300	-1.11651500
O	-2.22725000	-1.37840800	-0.11407300
C	-3.14729700	-1.30224500	-1.04444000
C	-2.92684500	-0.22908100	-2.12479500
H	-2.66169900	0.72265100	-1.64942000
H	-2.07488700	-0.52208000	-2.75537800
H	-3.82158400	-0.12259500	-2.74892600
O	-1.33624700	1.70218200	0.19427800
C	-2.02158900	2.08294400	1.24623000
O	-2.56603000	3.22992500	1.38588300
C	-2.15198000	1.04958200	2.37829300
H	-1.16049300	0.86446000	2.81454800
H	-2.83622200	1.41359800	3.15356900
H	-2.50281200	0.09780000	1.96162800
[Pd(OAc) ₂ (PhBr)] [±]			

Number of Imaginary Frequency = 1

Electronic Energy (Hartree) = -828.291899625

Tcg (Hartree) = 0.115839

DeltaG (solv kcal/mol) = -151.59

Charge = -2 Multiplicity = 1

C	-1.57028700	0.26046700	-0.00091300
Br	-2.26856300	-2.07108900	-0.27128800
C	-2.21378200	0.79596900	1.15924000
H	-2.12560800	0.25923700	2.09909600
C	-1.71225900	0.94524700	-1.26224600
C	-2.89927800	2.00828100	1.07316600
C	-3.00419600	2.71209900	-0.15989400
C	-2.41418900	2.17698600	-1.31157600
H	-3.34068400	2.43557600	1.97498500
H	-3.54502200	3.65712000	-0.20439000
H	-2.51552300	2.69265600	-2.26767400
H	-1.42400100	0.44355300	-2.18374600
Pd	0.36898600	0.24611200	-0.26970100
O	2.27639000	0.89630100	-1.13032600
O	1.24155500	-0.81311800	1.43223400
C	3.25693100	0.14909400	-1.58460200
C	1.88297600	-0.20566800	2.40791100
O	4.29192100	0.59582400	-2.18209400
C	3.09970100	-1.36640500	-1.38276400
O	2.39369100	-0.80294800	3.41191500

C	2.00256600	1.32308400	2.30344800
H	2.75310400	-1.57551800	-0.36416500
H	2.32810800	-1.74446000	-2.06871300
H	4.04619000	-1.87857600	-1.58899000
H	1.00150700	1.77188300	2.36189300
H	2.63086400	1.71098300	3.11331000
H	2.41986500	1.59110900	1.32524700

PhPd(OAc)₂Br

Number of Imaginary Frequency = 0

Electronic Energy (Hartree) = -828.366037721

Tcg (Hartree) = 0.118774

DeltaG (solv kcal/mol) = -148.62

Charge = -2 Multiplicity = 1

Pd	0.19234300	-0.02829600	-0.06503900
O	2.32368000	-0.00746700	-0.38890500
O	0.27447100	2.01211600	0.38444800
C	3.26756800	-0.21037400	0.49947200
C	0.68004200	2.96982200	-0.43374300
O	4.51693300	-0.17221000	0.25229300
C	2.78939700	-0.50947600	1.92843000
O	0.73083000	4.19231600	-0.09138100
C	1.08745800	2.54240100	-1.84349800
H	2.15576500	0.31619200	2.27591700
H	2.16969500	-1.41479800	1.91558800
H	3.64581800	-0.64088500	2.59945300
H	0.21986100	2.10573800	-2.35650500
H	1.45837700	3.40609900	-2.40603000
H	1.85217400	1.75939800	-1.77030300
C	-1.79538300	0.08824000	0.12099700
C	-2.34784000	1.01873600	1.03950700
C	-2.71098200	-0.69165300	-0.63163700
C	-3.73882500	1.14857800	1.21239400
H	-1.66644300	1.66605300	1.58579900
C	-4.10437500	-0.55194900	-0.47294800
H	-2.32219100	-1.43055900	-1.32734400
C	-4.63139200	0.36454400	0.45617800
H	-4.12557700	1.87467100	1.93000200
H	-4.77754800	-1.16968300	-1.07098900
H	-5.70986800	0.46804900	0.58500200
Br	0.12888200	-2.59571200	-0.32775300