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Supporting Information for:

Coupling of alkynols and a phenylate to a novel dihydronaphtalenide ligand on a ruthenium template

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Synthesis of compound 1a

In a typical run, 0.150 g (0.245 mmol) of [{(p-cymene)RuCl₂}₂] was reacted with 178 μ l (1.84 mmol) of 2-methyl-3-butyn-2-ol and 0.336 g (0.98 mmol) of NaBPh₄ in 8 ml of a 1:1 mixture of CH₂Cl₂ and MeOH. After stirring overnight, the reaction mixture was filtered by canula and the filtrate was evaporated to dryness in vacuum. The residue was dissolved in CH₂Cl₂, stirred for 45 min, and filtered again. The filtrate was evaporated under vacuum. The product was obtained as red powder and was washed 3x8 ml of Et₂O and dried in vacuum. Yield 69.4 % (0.132 g, 0.17mmol).

Compexes **2b,c** were prepared in an identical fashion and in yields of 66.2 and 71.5%, respectively.

Compound **2b:** ¹H-NMR (250 MHz, CD₂Cl₂), δ 1.32, 1.77 [each 3H, d CH₃(^{*i*}Pr), ³J_{H-H} = 6.88 Hz], 1.56-2.00 (m, 20H, CH₂), 1.80 [3H, s, CH₃(cym)], 1.95 [1H, s(br), OH] 2.14 [s, 3H, CH₃(cym)], 2.47 (1H, hept, CH(^{*i*}Pr), ³J_{H-H} = 6.88 Hz], 3.80 [1H, d, CH(cym), ³J_{H-H} = 6.2 Hz], 4.53 [1H, s, CH⁻], 4.70 [1H, d, CH(cym), ³J_{H-H} = 6.2 Hz], 4.88 [1H, d, CH(cym), ³J_{H-H} = 6.2 Hz], 5.05 [1H, d, CH(cym) ³J_{H-H} = 6.2 Hz], 6.40 [1H, s, CH(naph)], 7.33 [H, t, CH(naph), ³J_{H-H} = 7.20 Hz], 7.33, 7.34 [each 1H, t, CH(naph), ³J_{H-H} = 7.20 Hz], 7.47 [1H, t, CH(naph), ³J_{H-H} = 7.20 Hz], 7.48 [1H, m, CH(naph)]. ¹³C-NMR (250 MHz CD₂Cl₂), δ 16.13 [s, CH₃(cym)], 19.13 [s, CH₃(^{*i*}Pr)], 26.21, 27.35, 28.74, 38.36, 38.84, 39.13 [each s, CH₂(alc)], 32.51, 41.00 [s, CH(^{*i*}Pr)], 46.82 [s, CH⁻], 73.26 (s, C_q(alc)], 80.06, 86.4 [each s, C_q(cym)], 124.02, 127.95 [s, C=C(naph)], 130.55, 132.86, 131.01, 138.18 [s, CH (naph)]. CH analysis for C₅₄H₅₇BORu: calculated (measured): C 78.03 (77.37), H 7.13 (7.36).

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Compound **2c:** ¹H-NMR (250 MHz, CD₂Cl₂), δ 1.32, 1.77 [each 3H, d, ³J_{HH} = 6.88 Hz, CH₃(^{*i*}-Pr)], 1.56-2.00 [m, 16H, CH₂)] 1.85 [1H, broad, OH], 2.14 [3H, s, CH₃(cym)], 2.47 (1H, hept, CH(^{*i*}-Pr), ³J_{H-H} = 6.88 Hz], 3.98 [1H, d, CH(cym), ³J_{H-H} = 6.2 Hz], 4.34 [1H, s, CH⁻], 4.54, 4.80, 5.09 [each 1H, d, CH(cym) ³J_{HH} = 6.2 Hz], 6.66 [1H, s, CH(naph)], 7.33, 7.34, 7.47 [each 1H, t, CH(naph), ³J_{H-H} = 7.20 Hz], 7.48 [1H, m, CH(naph)]. ¹³C-NMR (250 MHz CD₂Cl₂) δ ¹³C-NMR (250 MHz CD₂Cl₂) δ 21.07 [s, CH₃(cym)], 24.06 [s, CH₃(^{*i*}Pr)], 26.20, 26.35, 27.51, 35.81 [each s, CH₂], 31.89 [s, CH₃(^{*i*}Pr)], 43.58 [s, CH(^{*i*}Pr)], 45.20 [s, CH⁻], 83.29 (s, <u>C</u>Me₂OH), 85.61 [s, C_q(naph)], 87.46 [s, C_q(naph]]. 88.70, 88.76, 89.83, 91.64 [s, CH(cym)], 106.58 [s, C_q(naph)], 113.54, 117.70 [each s, C_q(cym)], 125.86, 127.89 [each s, C=C(naph)], 129.21, 129.54, 130.48, 138.18 [each s, CH (naph)]. CH analysis for C₅₆H₆₁BORu: calculated (measured): C 77.78 (78.00), H 6.89 (6.91).



Figure S1: MS of 1a (positive ion CI, NH₃, 400K).

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Figure S2: Expanded section of S1, M^+ and base peak.



Figure S3: Comparison of experimental and simulated isotopic pattern of the base peak of **1a**.