Supporting Information
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Supporting Information for:

I₂ promoted metal-free head-to-tail dimerization of styrenes affording 1,3-diarylbut-1-enes

Dingyi Wang, Yanjiao Fang, Qihuang Xie, Sen Lin* and Shengmei Guo*

College of Chemistry, Nanchang University, Nanchang, Jiangxi 330031, P. R. China

General Information

¹H and ¹³C NMR spectra were recorded on Bruker Ascend™ 400(400 MHz) using tetramethylsilane as an internal reference. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, m = multiplet, br = broad signal. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively.

Chemicals were purchased from the Sinopharm Chemical Reagent Co., Adamas, Aladdin and TCI used as received.

General procedure for the preparation of the corresponding product 2.

P(OEt)₃ (0.20 mmol) was added to a solution of 1 (0.20 mmol) and I₂ (0.40 mmol) in DCE (1 mL), and the reaction mixture was stirred under reflux conditions for 5-30 min. After completion of the reaction, the reaction mixture was diluted with ethyl acetate, and quenched with saturated sodium thiosulfate solution and extracted twice with ethyl acetate (3 × 15 mL). The organic layer was washed with water and dried over anhyd. sodium sulfate. The solvent was evaporated in vacuo, and the residue was subjected to column chromatography using ethyl acetate in petroleum ether as the eluent to afford the pure target compound 2.

(E)-but-1-ene-1,3-diyldibenzene (2a)¹: colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 7.37-7.18 (m,10H), 6.41 (d, J = 4.0 Hz, 2H), 3.66-3.63 (m, 1H), 1.47 (d, J = 8.0 Hz, 3H).

(E)-2,2’-(but-1-ene-1,3-diyl)bis(chlorobenzene) (2b)²: colorless oil. ¹H NMR (400 MHz, CDCl₃): δ 7.51 (d, J = 8.0 Hz, 1H), 7.40-7.15 (m, 7H), 6.88 (d, J = 16.0 Hz, 1H), 6.39-6.33 (m, 1H), 4.25-4.22 (m, 1H), 1.50 (d, J = 4.0 Hz, 3H).

(E)-3,3’-(but-1-ene-1,3-diyl)bis(chlorobenzene) (2c)³: colorless oil. ¹H NMR (400 MHz, CDCl₃):
δ 7.34-7.12 (m, 8H), 6.34 (s, 2H), 3.62-3.60 (m, 1H), 1.45 (d, J = 4.0 Hz, 3H).

(E)-4,4′-(but-1-ene-1,3-diyl)bis(chlorobenzene) (2d): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.31-7.27 (m, 6H), 7.19 (d, J = 8.0 Hz, 2H), 6.33 (d, J = 4.0 Hz, 2H), 3.65-3.60 (m, 1H), 1.45 (d, J = 8.0 Hz, 3H).

(E)-4,4′-(but-1-ene-1,3-diyl)bis(fluorobenzene) (2e): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.32-7.28 (m, 2H), 7.25-7.19 (m, 2H), 7.02-6.95 (m, 4H), 6.36-6.22 (m, 2H), 3.63-3.59 (m, 1H), 1.44 (d, J = 8.0 Hz, 3H).

(E)-4,4′-(but-1-ene-1,3-diyl)bis(bromobenzene) (2f): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.45-7.40 (m, 4H), 7.26-7.12 (m, 4H), 6.29 (d, J = 16.0 Hz, 2H), 3.63-3.58 (m, 1H), 1.44 (d, J = 4.0 Hz, 3H).

(E)-4,4′-(but-1-ene-1,3-diyl)bis(4,1-phenylene) diacetate (2g): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.35 (d, J = 8.0 Hz, 2H), 7.27-7.25 (m, 2H), 7.03-7.00 (m, 4H), 6.41-6.27 (m, 2H), 3.65-3.62 (m, 1H), 2.29 (s, 6H), 1.45 (d, J = 4.0 Hz, 3H).

(E)-4,4′-(but-1-ene-1,3-diyl)bis(methylbenzene) (2h): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.26-7.08 (m, 8H), 6.40-6.29 (m, 2H), 3.61-3.58 (m, 1H), 2.33 (s, 6H), 1.44 (d, J = 4.0 Hz, 3H).

(E)-4,4′-(but-1-ene-1,3-diyl)bis(tert-butylbenzene) (2i): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.34-7.19 (m, 8H), 6.43-6.31 (m, 2H), 3.62-3.59 (m, 1H), 1.45 (d, J = 8.0 Hz, 3H), 1.31 (s, 18H).
1,1,3-trimethyl-3-phenyl-2,3-dihydro-1H-indene (2m): colorless oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 7.28-7.11 (m, 9H), 2.43 (d, $J = 12.0$ Hz, 1H), 2.20 (d, $J = 12.0$ Hz, 1H), 1.69 (s, 3H), 1.35 (s, 3H), 1.03 (s, 3H).
