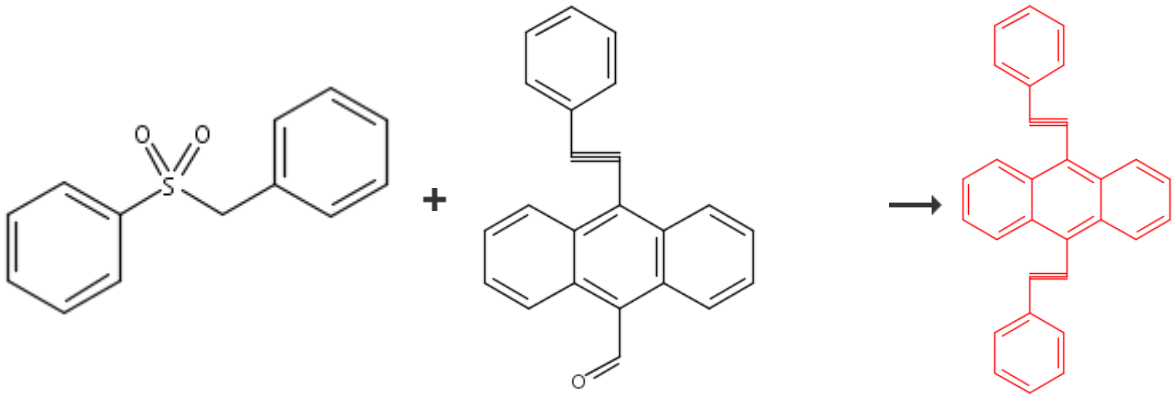
1. Single Step



98%

Overview

Steps/Stages

1.1 R:$(Me_3Si)_2NH$ •Li, R:$(EtO)_2P(=O)Cl$, S:THF, 0°C; 10 min, 0°C; 20 h, rt

1.2 R:NH_4Cl, S:H_2O

Notes

double elimination, 94% yield over 2 steps from 10-bromo-9-anthracenecarbaldehyde, alternative preparation shown, Reactants: 2, Reagents: 3, Solvents: 2, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Efficient synthesis of 9,10-bis(phenylethynyl)anthracene derivatives by integration of sonogashira coupling and double-elimination reactions

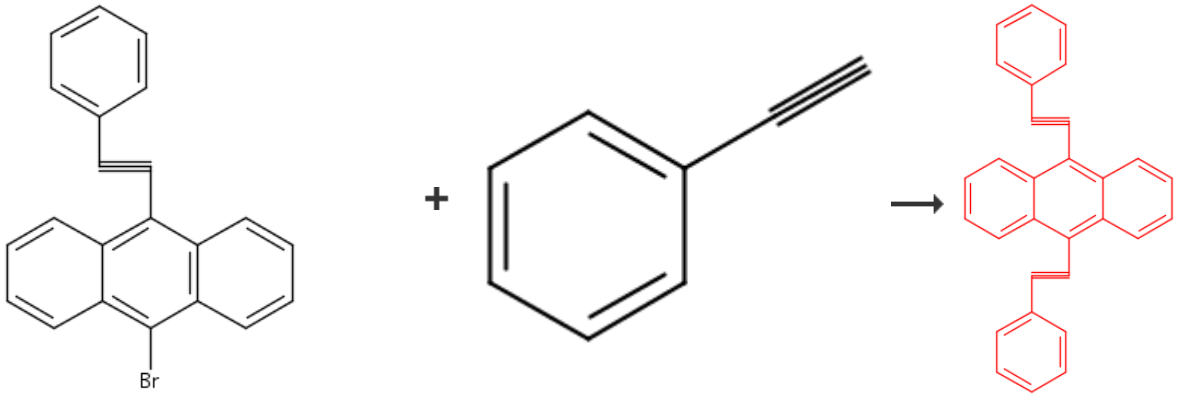
By Toyota, Shinji et al

From Synthesis, 45(8), 1060-1068; 2013

Experimental Procedure

General/Typical Procedure: To a soln of 5 (114 mg, 0.40 mmol), benzyl phenyl sulfone (7a) (112 mg, 0.48 mmol), and DECP (70 μL, 0.48 mmol) in anhyd THF (12 mL) was slowly added the LiHMDS soln (2.0 mL, 2.0 mmol) with a syringe at 0 °C under argon. This solution was stirred at 0 °C for 10 min, and then at r.t. for 20 h (reaction mixture B). The reaction was quenched with aq NH_4Cl (12 mL), and the organic materials were extracted with $CHCl_3$ (3 × 20 mL). The combined organic solution was dried over $MgSO_4$ and concentrated. The residue was recrystallized (hexane-$CHCl_3$). 9,10-Bis(phenylethynyl)anthracene (1a). This compound was synthesized by DE with 8a (123 mg, 0.40 mmol) and 7a (112 mg, 0.48 mmol) according to the typical procedure. The formed solid was collected by filtration, washed with water, and dried. Recrystallization (hexane-$CHCl_3$) gave the desired product. Yield: 148 mg (98%). mp 242-248 °C (dec) (Lit. 257-258 °C, Lit. 253 °C, Lit. 249-250 °C). This sample slowly decomposed >240 °C and showed a sharp endothermic peak at 258 °C on DTA measurement. R_f = 0.41 (hexane-$CHCl_3$, 4:1). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.40-7.48 (m, 6 H), 7.66 (m, 4 H), 7.78 (dd, *J*= 1.6, 8.0 Hz, 4 H), 8.70 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 86.4, 102.4, 118.5, 123.3, 126.8, 127.2, 128.6, 128.7, 131.7, 132.1. UV/Vis ($CHCl_3$): λ_{max} (ε) = 275 (105000), 313 (43300), 439 (38900), 464 nm (41000). FL ($CHCl_3$): λ_{max} = 475, 506 nm (λ_{max} 458 nm, Φ_f 0.81, τ_f 2.5 ns).

2. Single Step



93%

Overview

Steps/Stages

1.1 R:Et_3N, C:CuI, C:$PdCl_2(PPh_3)_2$, S:THF, 2 h, 70°C

Notes

84% yield over 2 steps from 10-bromo-9-anthracenecarbaldehyde, Sonogashira coupling, alternative preparation shown, Reactants: 2, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Efficient synthesis of 9,10-bis(phenylethynyl)anthracene derivatives by integration of sonogashira coupling and double-elimination reactions

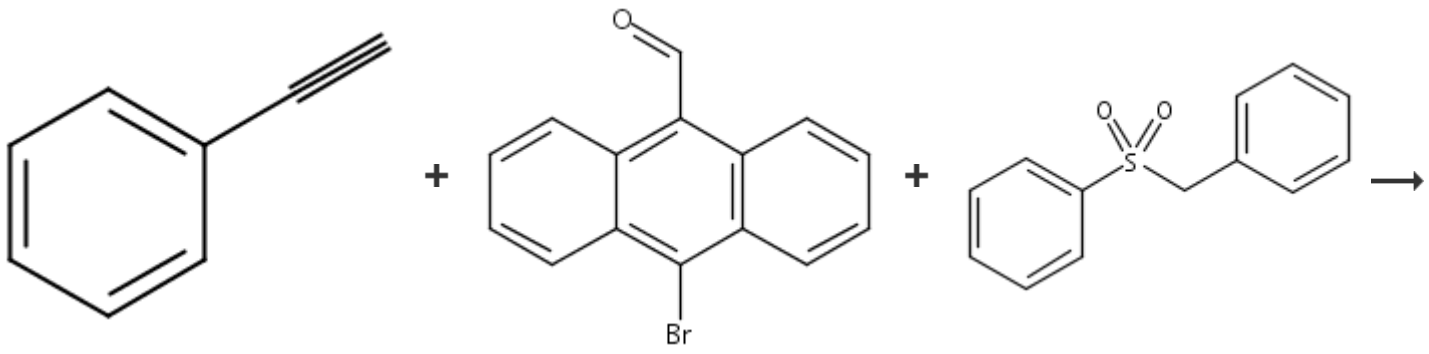
By Toyota, Shinji et al

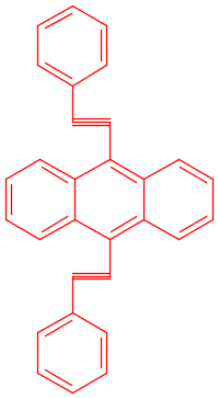
From Synthesis, 45(8), 1060-1068; 2013

Experimental Procedure

10-(Phenylethynyl)-9-anthracenecarbaldehyde (8a); Typical Procedure for SC. To a soln of 10-bromo-9-anthracenecarbaldehyde (5) (114 mg, 0.40 mmol) and phenylethyne (6a) (49 mg, 0.48 mmol) in a degassed mixture of anhyd THF (8 mL) and Et_3N (8 mL) were added[$PdCl_2(PPh_3)_2$] (11 mg, 16 μmol) and CuI (6.1 mg, 32 μmol). The reaction mixture was stirred at 70 °C for 2 h under argon (reaction mixture A). The solvent was removed, and the crude product was purified by chromatography on silica gel (hexane-$CHCl_3$, 10:1). The same compound was also synthesized by SC with 9a (143 mg, 0.40 mmol) and 6a (49 mg, 0.48 mmol) by the typical procedure. Chromatographic purification (hexane-$CHCl_3$, 10:1) gave 1a; yield: 141 mg (93%).

3. Single Step





90%

Overview

Steps/Stages

1.1 R:Et_3N, C:CuI, C:$PdCl_2(PPh_3)_2$, S:THF, 2 h, 70°C

1.2 R:$(Me_3Si)_2NH$ •Li, R:$(EtO)_2P(=O)Cl$, S:THF, 0°C; 10 min, 0°C; 20 h, rt

1.3 R:NH_4Cl, S:H_2O

Notes

double elimination (stage 2), alternative reaction conditions gave lower yield, alternative preparation shown, Sonogashira coupling (stage 1), Reactants: 3, Reagents: 4, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 3, Most stages in any one step: 3

References

Efficient synthesis of 9,10-bis(phenylethynyl)anthracene derivatives by integration of sonogashira coupling and double-elimination reactions

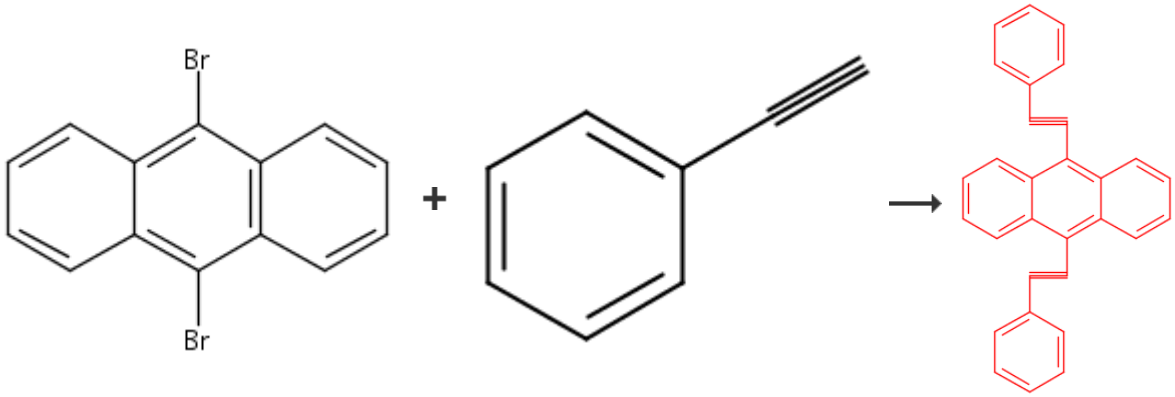
By Toyota, Shinji et al

From Synthesis, 45(8), 1060-1068; 2013

Experimental Procedure

To a soln of 10-bromo-9-anthracenecarbaldehyde (5) (114 mg, 0.40 mmol) and phenylethyne (6a) (49 mg, 0.48 mmol) in a degassed mixture of anhyd THF (8 mL) and Et_3N (8 mL) were added [$PdCl_2(PPh_3)_2$] (11 mg, 16 μmol) and CuI (6.1 mg, 32 μmol). The reaction mixture was stirred at 70 °C for 2 h under argon (reaction mixture A). The solvent was removed, and the crude product was purified by chromatography on silica gel (hexane-$CHCl_3$, 10:1). 9-Bromo-10-(phenylethynyl)anthracene (9a); Typical Procedure for One-Shot DE. To a soln of 5 (114 mg, 0.40 mmol), benzyl phenyl sulfone (7a) (112 mg, 0.48 mmol), and DECP (70 μL, 0.48 mmol) in anhyd THF (12 mL) was slowly added the LiHMDS soln (2.0 mL, 2.0 mmol) with a syringe at 0 °C under argon. This solution was stirred at 0 °C for 10 min, and then at r.t. for 20 h (reaction mixture B). The reaction was quenched with aq NH_4Cl (12 mL), and the organic materials were extracted with $CHCl_3$ (3 × 20 mL). The combined organic solution was dried over $MgSO_4$ and concentrated. The residue was recrystallized (hexane-$CHCl_3$). yellow crystals. Yield: 129 mg (90%). mp 167-169 °C (Lit. 170-171 °C). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.44-7.49 (m, 3 H), 7.63-7.66 (m, 4 H), 7.78 (dd, *J*= 8.0, 1.6 Hz, 2 H), 8.57 (m, 2 H), 8.72 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 86.0, 101.8, 118.2, 123.4, 124.2, 126.8, 127.2, 127.4, 128.2, 128.6, 128.8, 130.2, 131.6, 133.0.

4. Single Step



84%

Overview

Steps/Stages

1.1 R:*i*-Pr_2NH, C:$Pd(PPh_3)_4$, C:CuI, S:THF, 4.5 h, 80°C

Notes

Sonogashira coupling, sealed flask used, Reactants: 2, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Why Triple Bonds Protect Acenes from Oxidation and Decomposition

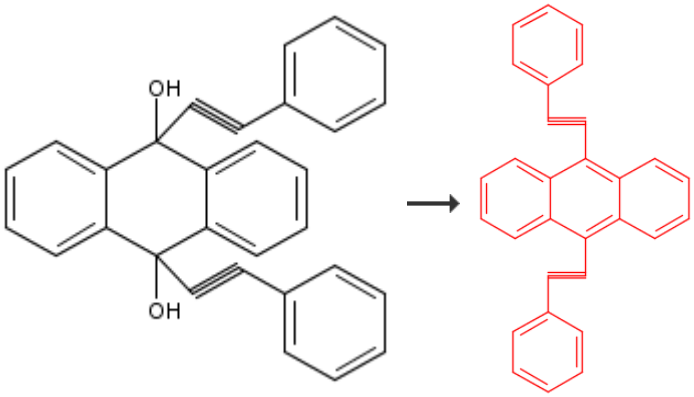
By Fudickar, Werner and Linker, Torsten

From Journal of the American Chemical Society, 134(36), 15071-15082; 2012

Experimental Procedure

Synthesis of arylalkynylanthracenes 1a-e: General procedure for the syntheses of arylalkynylanthracenes 1a-c. METHOD A: Dibromoanthracene (336 mg, 1 mmol), $[Pd(PPh_3)_2Cl_2]$ (60 mg, 0.08 mmol) and CuI (100 mg, 0.52 mmol) were placed in a round bottom flask and dissolved in dry THF (8 mL) and dry *i*Pr_2NH (8 mL). After degassing by three freeze-pump-thaw cycles the flask was filled with argon and sealed with a septum. At 80 °C the arylacetylene (2.1 mmol) was added neat *via* syringe pump over a period of 4.5 h. Thereafter, the solvent was evaporated and the residue was suspended in methanol. The precipitate was filtered and the residue was dissolved in hot $CHCl_3$. After hot filtration the product precipitated upon cooling. **9,10-Bis(phenylethynyl)anthracene (1a)**, yield 315 mg, 84%, orange crystals. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.41-7.51(6H, m, ArH-3, ArH-4, ArH-5), 7.66 (4H, dd, *J*=3.2 Hz, 5.6 Hz, H-2, H-3, H-6, H-7), 7.83 (4H, dd, *J*=6.1 Hz, 7.9 Hz, ArH-2, ArH-6), 8.71 (4H, dd, *J*=3.2 Hz, 5.6 Hz, H-1, H-4, H-5, H-8). ^{13}C NMR (60 MHz, $CDCl_3$): δ(s, AlkynylC-2), 102.4 (s, AlkynylC-1), 118.5 (s, C-9, C-10), 123.4 (s, ArC-1), 126.8 (d, C-2, C-3, C-6, C-7), 127.2 (d, C-1, C-4, C-5, C-8), 128.5 (d, ArC-3, ArC-5), 128.6 (d, ArC-4), 131.7 (d, ArC-2, ArC-6), 132.1 (s, C-11, C-12, C-13, C-14). Mp 263 °C. IR (cm^{-1}, ATR): ν = 2962, 2196, 1672, 1594, 1451, 1400, 1331, 1305, 1281, 1255. MS (EI): 378 [M^+]. Elemental analysis calcd (%) for $C_{30}H_{18}$ (378.47): C 95.21, H 4.79; found: C 94.96, H 4

5. Single Step



100%

Overview

Steps/Stages

1.1 $R:SnCl_2$

Notes

Reactants: 1, Reagents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

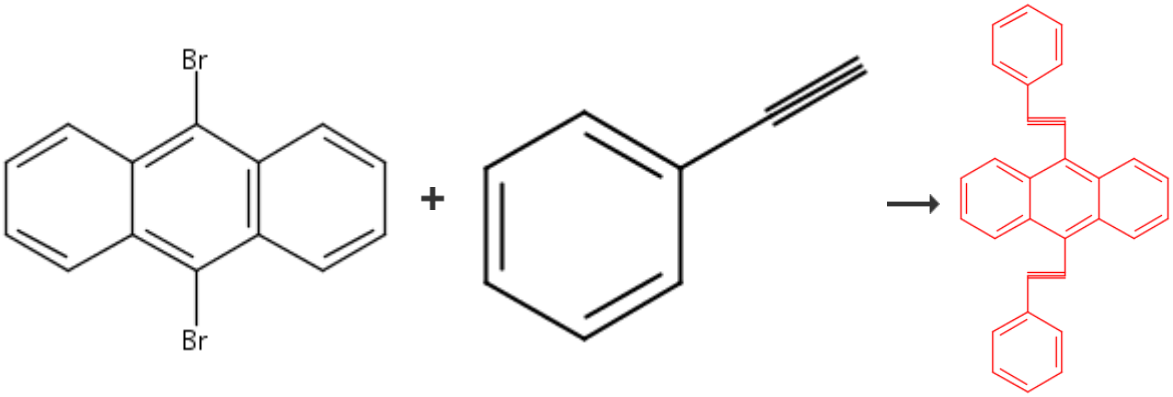
References

Synthesis of derivatives of 9,10-bis(phenylethynyl)anthracene

By Kutikova, G. A. et al

From Sbornik Nauchnykh Trudov - Vsesoyuznyi Nauchno-Issledovatel'skii Institut Lyuminoforov i Osobo Chistykh Veshchestv, 28, 86-92; 1985

6. Single Step



84%

Overview

Steps/Stages

Notes

1.1 C:CuI, C:$PdCl_2(PPh_3)_2$, S:THF, S:*i*-Pr_2NH, 4.5 h, 80°C

sealed flask used, syringe pump used, Sonogashira reaction, Reactants: 2, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Reversible Photooxygenation of Alkynylanthracenes: Chemical Generation of Singlet Oxygen under Very Mild Conditions

By Fudickar, Werner and Linker, Torsten

From Chemistry - A European Journal, 17(49), 13661-13664, S13661/1-S13661/24; 2011

Reaction Protocol

Procedure

1. Place dibromoanthracene (336 mg, 1 mmol), [$Pd(PPh_3)_2Cl_2$] (60 mg, 0.08 mmol) and CuI (100 mg, 0.52 mmol) in a round bottom flask.
2. Dissolve the mixture in dry THF (8 mL) and dry iPr_2NH (8 mL).

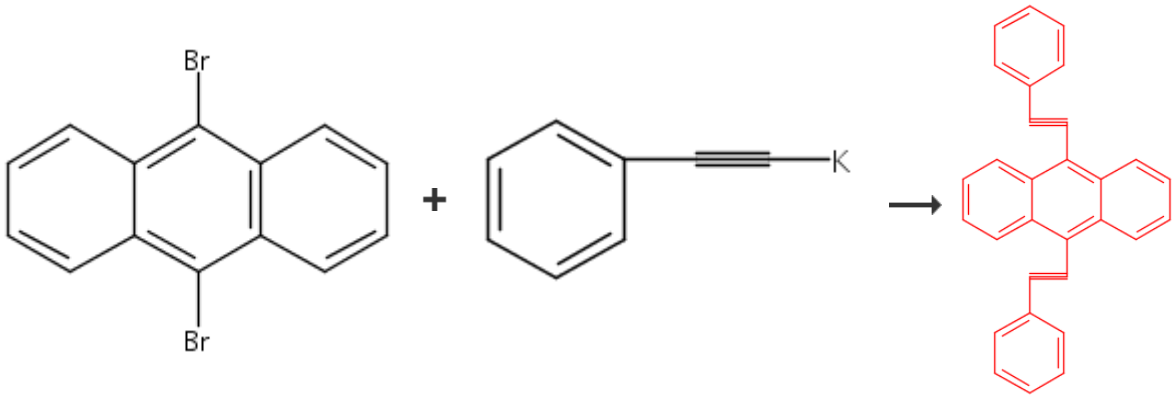
View more...

Available Experimental Data

^1H NMR, ^{13}C NMR, IR, Elemental Analysis, Mass Spec, MP, State

View with MethodsNow

7. Single Step



85%

Overview

Steps/Stages **Notes**

1.1 C:9-BBN-OMe, C:72287-26-4, S:THF

Reactants: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

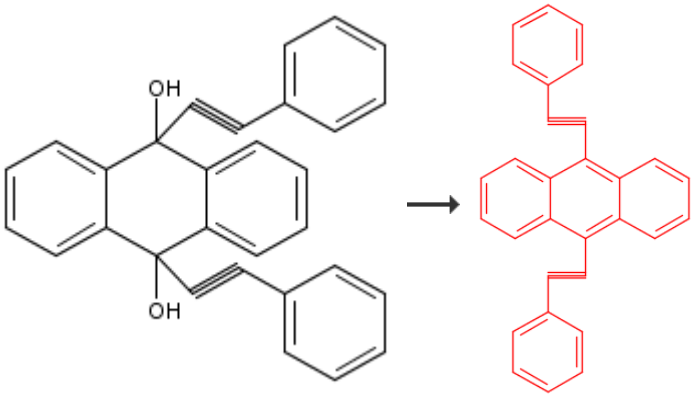
References

Palladium-catalyzed arylation of polar organometallics mediated by 9-methoxy-9-borabicyclo[3.3.1]nonane: Suzuki reactions of extended scope

By Fuerstner, Alois and Seidel, Guenter

From Tetrahedron, 51(41), 11165-76; 1995

8. Single Step



100%

Overview

Steps/Stages

1.1 R:HI, S:H_2O, S:Et_2O

Notes

Classification: Aromatisation; Dehydroxylation; # Conditions: HI H2O Et2O ; 20 s, Reactants: 1, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

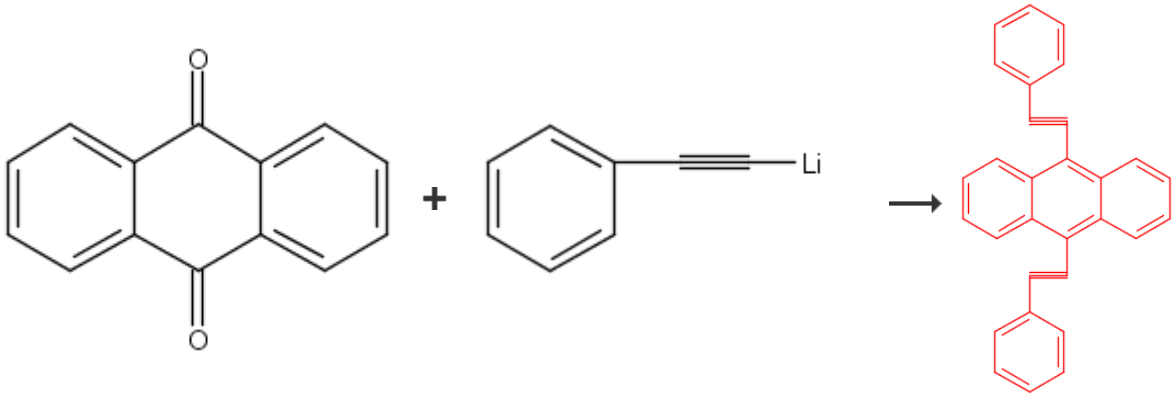
References

A study of transannular rearrangements in the 9,10-bis-(phenylethynyl)anthracene series

By Rio, Guy

From Ann. chim. (Paris), 9, 182-255; 1954

9. Single Step



72%

Overview

Steps/Stages

1.1 S:THF, -78°C; 5 h, cooled

1.2 R:NH_4Cl, S:H_2O

1.3 R:$SnCl_2$ •$2H_2O$, S:THF, 30 min

Notes

regioselective, excess lithium acetylide used, Reactants: 2, Reagents: 2, Solvents: 2, Steps: 1, Stages: 3, Most stages in any one step: 3

References

Synthesis and characterization of solution processable 6,11-dialkynyl substituted indeno[1,2-b]anthracenes

By Yucel, Baris et al

From Dyes and Pigments, 100, 104-117; 2014

Reaction Protocol

Procedure

1. Add n-BuLi (4.20 mL of a 1.6 M of hexane solution, 6.72 mmol, 2.8 eq.) to a solution of phenylacetylene (0.86 g, 8.40 mmol, 3.5 eq.) in THF (15 mL) Cool to -78°C dropwise.
2. Allow the solution to stir for 30 min.

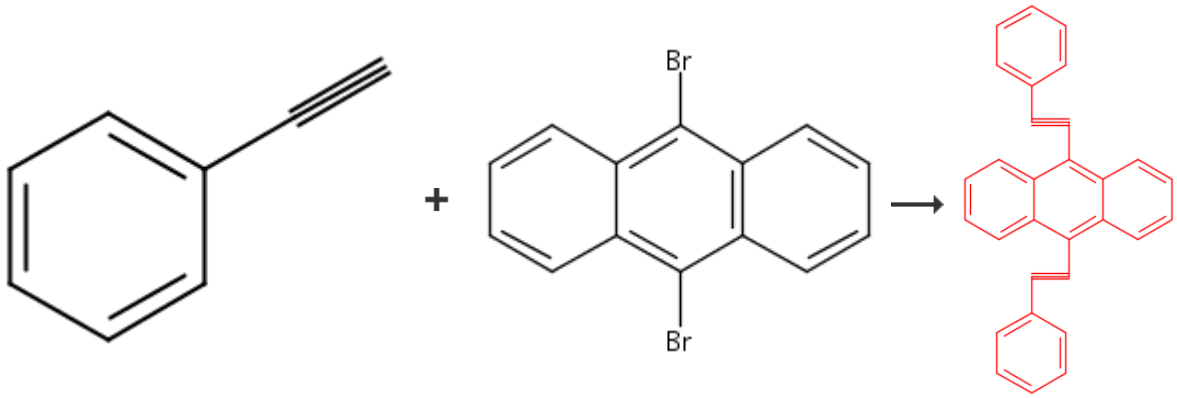
View more...

Available Experimental Data

State

View with MethodsNow

10. Single Step



71%

Overview

Steps/Stages

1.1 R:BuLi, S:THF, S:$Me(CH_2)_4Me$, -78°C; 10 min, -78°C; -78°C → rt

1.2 R:$InCl_3$, S:THF, -78°C; 30 min, -78°C; 30 min, -78°C → rt

1.3 C:72287-26-4, S:THF, 24 h, 70°C; 70°C → rt

1.4 R:$NaHCO_3$, S:H_2O, rt

Notes

Reactants: 2, Reagents: 3, Catalysts: 1, Solvents: 3, Steps: 1, Stages: 4, Most stages in any one step: 4

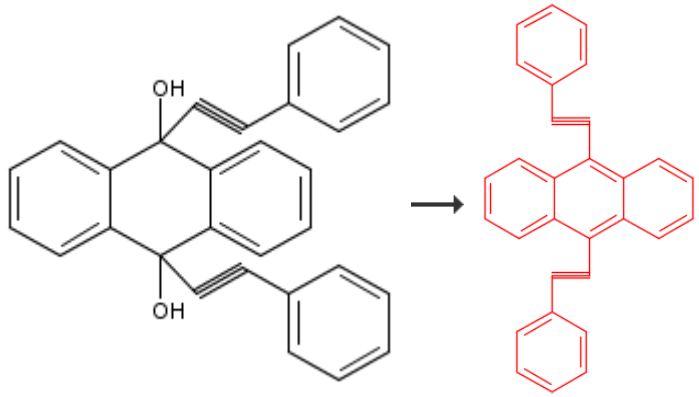
References

Palladium-Catalyzed Multialkynyl Cross-Coupling Reactions with Tetraalkynylindates

By Kang, Dongjin et al

From European Journal of Organic Chemistry, (12), 2330-2336; 2010

11. Single Step



65%

Overview

Steps/Stages

Notes

1.1 R:$SnCl_2$ •$2H_2O$, R:AcOH, S:H_2O, S:EtOH, 10 min, 60°C

Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

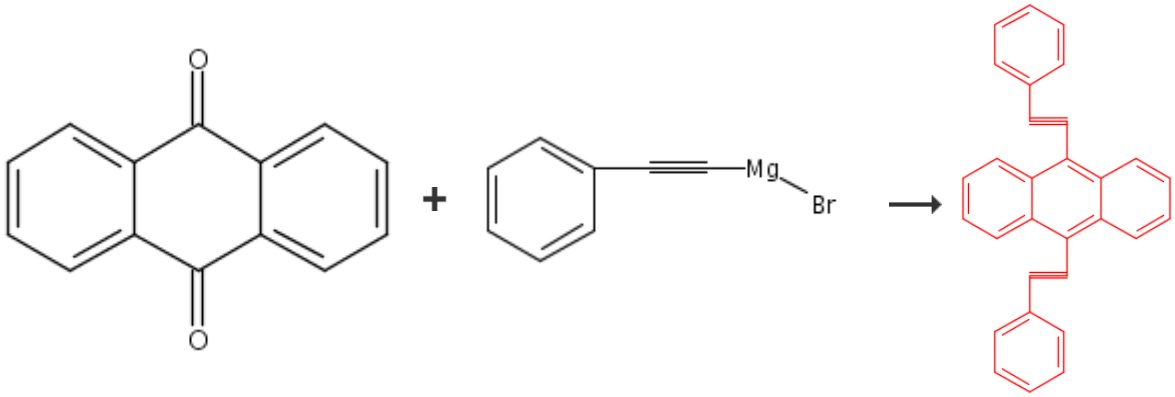
References

A simple "palladium-free" synthesis of phenyleneethynylene-based molecular materials revisited

By Lydon, Donocadh P. et al

From New Journal of Chemistry, 29(7), 972-976; 2005

12. Single Step



Overview

Steps/Stages

1.1 S:Dioxane

1.2 R:$SnCl_2$

Notes

Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

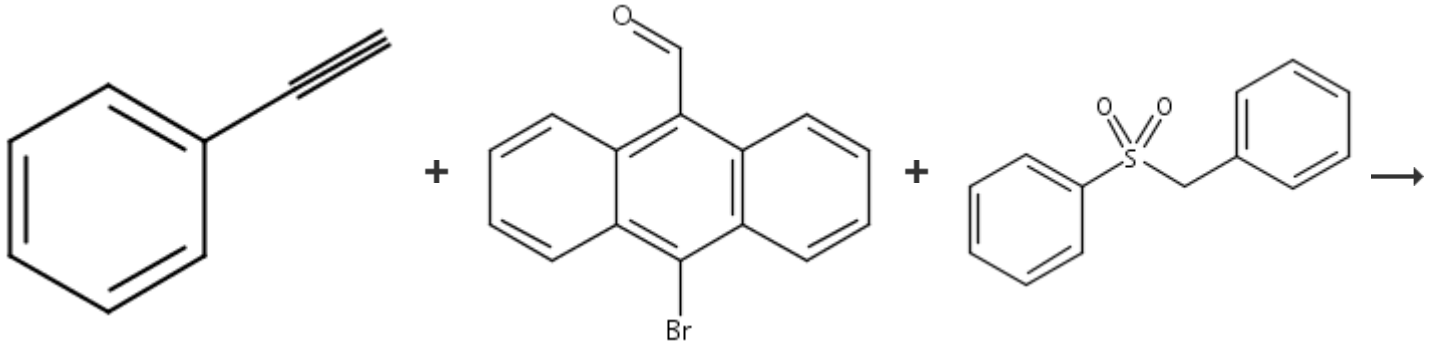
References

Preparation of 9,10-bis(phenylethynyl)anthracene and its chloro derivatives

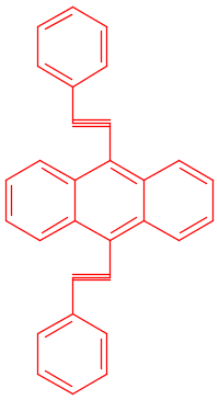
By Krasovitskij, B. M. et al

From U.S.S.R., 1031103, 28 Feb 1993

13. 2 Steps



[Step 2.1]



Overview

Steps/Stages

1.1 R:Et_3N, C:CuI, C:$PdCl_2(PPh_3)_2$, S:THF, 2 h, 70°C

2.1 R:$(Me_3Si)_2NH$ •Li, R:$(EtO)_2P(=O)Cl$, S:THF, 0°C; 10 min, 0°C; 20 h, rt

2.2 R:NH_4Cl, S:H_2O

Notes

1) Sonogashira coupling, 2) double elimination, 94% yield over 2 steps from 10-bromo-9-anthracenecarbaldehyde, alternative preparation shown, Reactants: 3, Reagents: 4, Catalysts: 2, Solvents: 2, Steps: 2, Stages: 3, Most stages in any one step: 2

References

Efficient synthesis of 9,10-bis(phenylethynyl)anthracene derivatives by integration of sonogashira coupling and double-elimination reactions

By Toyota, Shinji et al

From Synthesis, 45(8), 1060-1068; 2013

Experimental Procedure

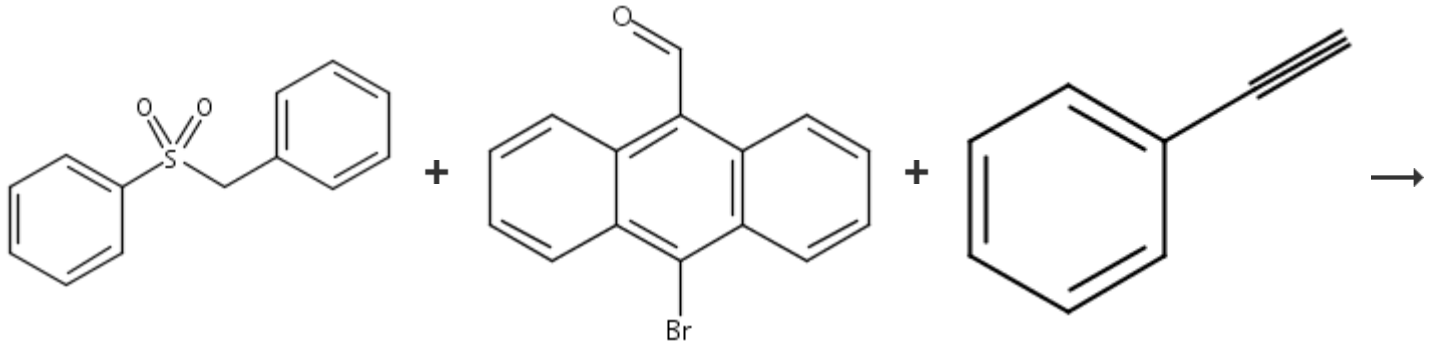
Step 1

General/Typical Procedure: 10-(Phenylethynyl)-9-anthracenecarbaldehyde (8a); Typical Procedure for SC. To a soln of 10-bromo-9-anthracenecarbaldehyde (5) (114 mg, 0.40 mmol) and phenylethyne (6a) (49 mg, 0.48 mmol) in a degassed mixture of anhyd THF (8 mL) and Et_3N (8 mL) were added[$PdCl_2(PPh_3)_2$] (11 mg, 16 µmol) and CuI (6.1 mg, 32 µmol). The reaction mixture was stirred at 70 °C for 2 h under argon (reaction mixture A). The solvent was removed, and the crude product was purified by chromatography on silica gel (hexane-$CHCl_3$, 10:1). as an orange solid. Yield: 117 mg (96%). mp 198-200 °C (Lit. 179-180 °C); R_f = 0.26 (hexane-$CHCl_3$, 4:1). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.48-7.53 (m, 3 H), 7.65-7.74 (m, 4 H), 7.79-7.82 (m, 2 H), 8.79 (d, *J*= 8.7 Hz, 2 H), 8.97 (d, *J*= 8.7 Hz, 2 H), 11.53 (s, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 86.1, 104.6, 122.8, 123.8, 124.9, 125.5, 126.5, 127.6, 128.6, 128.9, 129.2, 131.1, 131.7, 131.8, 192.9.

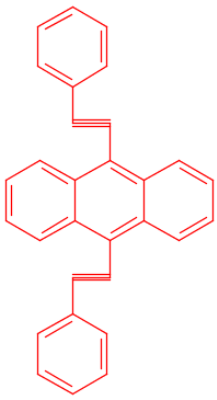
Step 2

General/Typical Procedure: To a soln of 5 (114 mg, 0.40 mmol), benzyl phenyl sulfone (7a) (112 mg, 0.48 mmol), and DECP (70 µL, 0.48 mmol) in anhyd THF (12 mL) was slowly added the LiHMDS soln (2.0 mL, 2.0 mmol) with a syringe at 0 °C under argon. This solution was stirred at 0 °C for 10 min, and then at r.t. for 20 h (reaction mixture B). The reaction was quenched with aq NH_4Cl (12 mL), and the organic materials were extracted with $CHCl_3$ (3 × 20 mL). The combined organic solution was dried over $MgSO_4$ and concentrated. The residue was recrystallized (hexane-$CHCl_3$). 9,10-Bis(phenylethynyl)anthracene (1a). This compound was synthesized by DE with 8a (123 mg, 0.40 mmol) and 7a (112 mg, 0.48 mmol) according to the typical procedure. The formed solid was collected by filtration, washed with water, and dried. Recrystallization (hexane-$CHCl_3$) gave the desired product. Yield: 148 mg (98%). mp 242-248 °C (dec) (Lit. 257-258 °C, Lit. 253 °C, Lit. 249-250 °C). This sample slowly decomposed >240 °C and showed a sharp endothermic peak at 258 °C on DTA measurement. R_f = 0.41 (hexane-$CHCl_3$, 4:1). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.40-7.48 (m, 6 H), 7.66 (m, 4 H), 7.78 (dd, *J*= 1.6, 8.0 Hz, 4 H), 8.70 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 86.4, 102.4, 118.5, 123.3, 126.8, 127.2, 128.6, 128.7, 131.7, 132.1. UV/Vis ($CHCl_3$): λ_{max} (ε) = 275 (105000), 313 (43300), 439 (38900), 464 nm (41000). FL ($CHCl_3$): λ_{max} = 475, 506 nm (λ_{max} 458 nm, Φ_f 0.81, τ_f 2.5 ns).

14. 2 Steps



[Step 2.1]



Overview

Steps/Stages **Notes**

1.1 R:$(Me_3Si)_2NH$ •Li, R:$(EtO)_2P(=O)Cl$, S:THF, 0°C; 10 min, 0°C; 20 h, rt

1.2 R:NH_4Cl, S:H_2O

2.1 R:Et_3N, C:CuI, C:$PdCl_2(PPh_3)_2$, S:THF, 2 h, 70°C

1) double elimination, 2) 84% yield over 2 steps from 10-bromo-9-anthracenecarbaldehyde, Sonogashira coupling, alternative preparation shown, Reactants: 3, Reagents: 4, Catalysts: 2, Solvents: 2, Steps: 2, Stages: 3, Most stages in any one step: 2

References

Efficient synthesis of 9,10-bis(phenylethynyl)anthracene derivatives by integration of sonogashira coupling and double-elimination reactions

By Toyota, Shinji et al

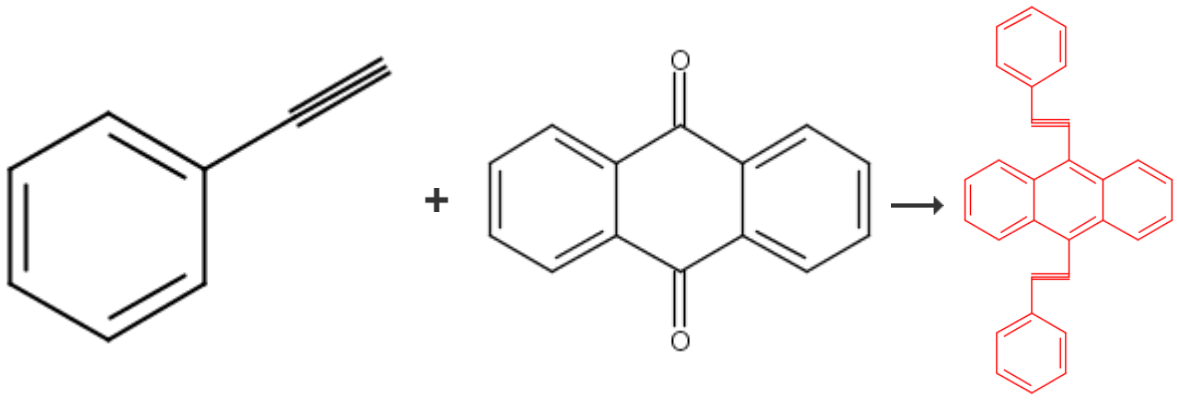
From Synthesis, 45(8), 1060-1068; 2013

Experimental Procedure

Step 1
To a soln of 5 (114 mg, 0.40 mmol), benzyl phenyl sulfone (7a) (112 mg, 0.48 mmol), and DECP (70 µL, 0.48 mmol) in anhyd THF (12 mL) was slowly added the LiHMDS soln (2.0 mL, 2.0 mmol) with a syringe at 0 °C under argon. This solution was stirred at 0 °C for 10 min, and then at r.t. for 20 h (reaction mixture B). The reaction was quenched with aq NH_4Cl (12 mL), and the organic materials were extracted with $CHCl_3$ (3 × 20 mL). The combined organic solution was dried over $MgSO_4$ and concentrated. The residue was recrystallized (hexane-$CHCl_3$). One-Pot Synthesis of 1b. This reaction was carried out with reaction mixture A and 7b (118 mg, 0.48 mmol). The crude product was purified by chromatography on silica gel (hexane-$CHCl_3$, 10:1) to give the pure product; yield: 141 mg (90%).

Step 2
10-(Phenylethynyl)-9-anthracenecarbaldehyde (8a); Typical Procedure for SC. To a soln of 10-bromo-9-anthracenecarbaldehyde (5) (114 mg, 0.40 mmol) and phenylethyne (6a) (49 mg, 0.48 mmol) in a degassed mixture of anhyd THF (8 mL) and Et_3N (8 mL) were added[$PdCl_2(PPh_3)_2$] (11 mg, 16 µmol) and CuI (6.1 mg, 32 µmol). The reaction mixture was stirred at 70 °C for 2 h under argon (reaction mixture A). The solvent was removed, and the crude product was purified by chromatography on silica gel (hexane-$CHCl_3$, 10:1). The same compound was also synthesized by SC with 9a (143 mg, 0.40 mmol) and 6a (49 mg, 0.48 mmol) by the typical procedure. Chromatographic purification (hexane-$CHCl_3$, 10:1) gave 1a; yield: 141 mg (93%).

15. 2 Steps



Overview

Steps/Stages **Notes**

1.1 R:BuLi, S:THF, -70°C; -70°C → rt; rt → -70°C
1.2 S:THF, -70°C → rt; overnight, rt

1.3 R:NH_4Cl, S:H_2O, 0°C

2.1 R:$SnCl_2$ •$2H_2O$, R:AcOH, S:H_2O, S:EtOH, 10 min, 60°C

Reactants: 2, Reagents: 4, Solvents: 3, Steps: 2, Stages: 4, Most stages in any one step: 3

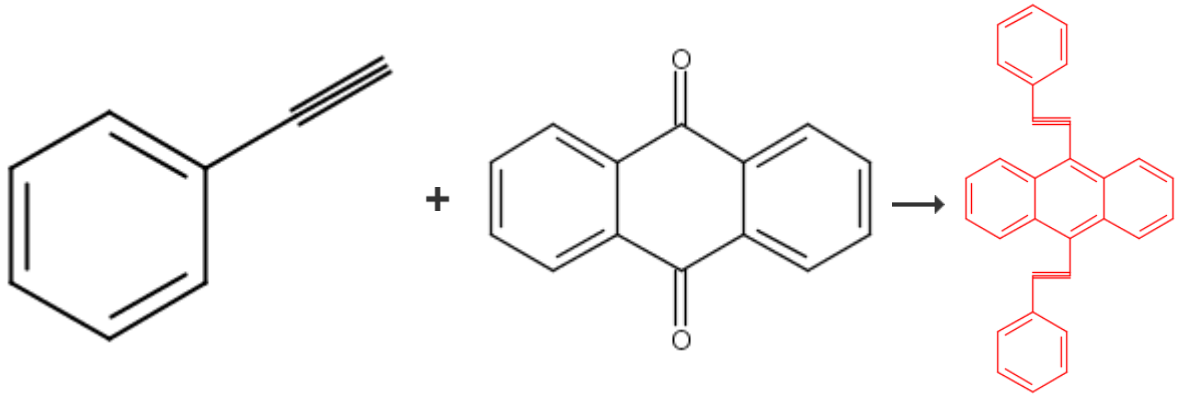
References

A simple "palladium-free" synthesis of phenyleneethynylene-based molecular materials revisited

By Lydon, Donocadh P. et al

From New Journal of Chemistry, 29(7), 972-976; 2005

16. 2 Steps



Overview

Steps/Stages

1.1 C:EtMgI

2.1 R:$SnCl_2$

Notes

Reactants: 2, Reagents: 1, Catalysts: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

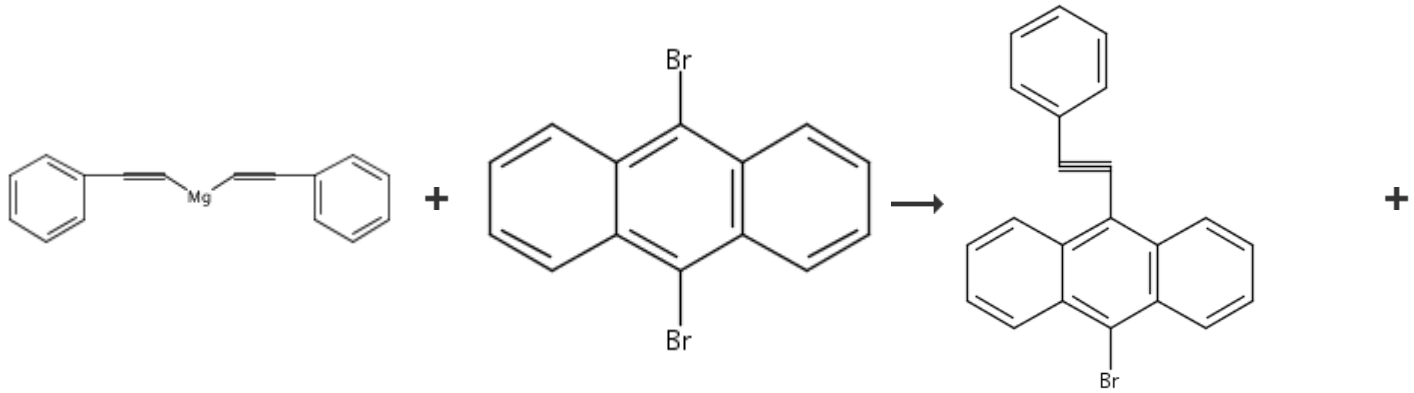
References

Synthesis of derivatives of 9,10-bis(phenylethynyl)anthracene

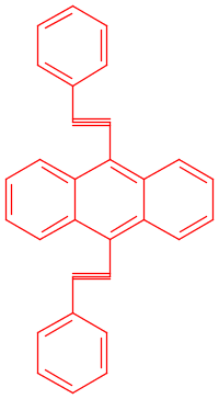
By Kutikova, G. A. et al

From Sbornik Nauchnykh Trudov - Vsesoyuznyi Nauchno-Issledovatel'skii Institut Lyuminoforov i Osobo Chistykh Veshchestv, 28, 86-92; 1985

17. Single Step



78% (**25**:75)



78% (25:**75**)

Overview

Steps/Stages

1.1 C:Pd acetylacetonate, C:PPh_3, S:THF

Notes

Reactants: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

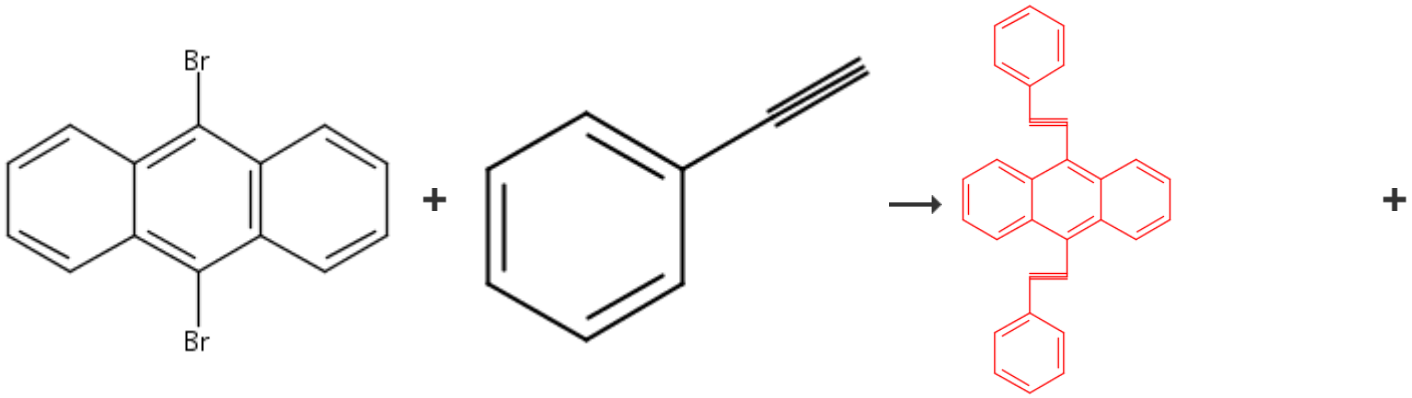
References

Cross-coupling of magnesium diacetylides with organic halides catalyzed by transition metal complexes

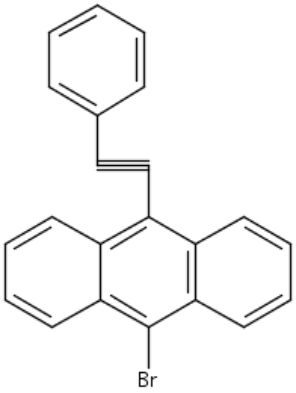
By Dzhemilev, U. M. et al

From Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (9), 2037-41; 1987

18. Single Step



52%



48%

Overview

Steps/Stages

1.1 R:*i*-Pr_2NH, C:$Pd(PPh_3)_4$, C:CuI, S:PhMe, 17 h, 80°C

Notes

Sonogashira coupling, Reactants: 2, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

De novo design for functional amorphous materials: Synthesis and thermal and light-emitting properties of twisted anthracene-functionalized bimesitylenes

By Moorthy, Jarugu Narasimha et al

From Journal of the American Chemical Society, 130(51), 17320-17333; 2008

Experimental Procedure

9-Bromo-10-phenylethynylanthracene (17). [2] Yield 48%; mp 169-170 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45(m, 3H), 7.63 (m, 4H), 7.77 (m, 2H), 8.57 (m, 2H), 8.69 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 85.9, 101.7, 118.2, 123.3, 124.1, 126.8, 127.2, 127.4, 128.2, 128.5, 128.7, 130.2, 131.6, 132.9.