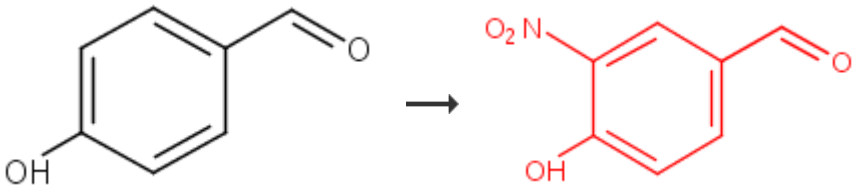
1. Single Step



94%

Overview

Steps/Stages

1.1 R:$Zn(NO_3)_2$, S:$HOCH_2CH_2OH$ polymer, S:H_2O, 3-4 min

Notes

green chemistry, green chemistry-solvent, regioselective, microwave irradiation, alternative reaction conditions shown, Reactants: 1, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

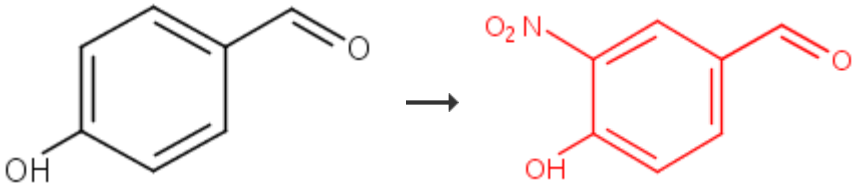
References

Ultrasonic and microwave effects in polyethylene glycol-bound metal nitrate initiated nitration of aromatic compounds under acid free conditions

By Rajanna, K. C. et al

From Green Chemistry Letters and Reviews, 8(3-4), 50-55; 2015

2. Single Step

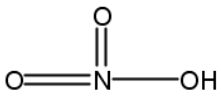


98%

Overview

Steps/Stages

1.1 R:



- 1/2 Mg

- 3 H_2O

R:Al_2O_3, R:$MeSO_3H$, > 1 min

1.2 35 min, rt

Notes

regioselective, safety-nitrated products are potential carcinogens, no solvent, Reactants: 1, Reagents: 3, Steps: 1, Stages: 2, Most stages in any one step: 2

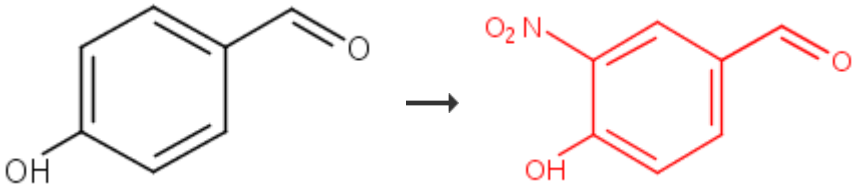
References

Al2O3/MeSO3H (AMA) as a novel heterogeneous system for the nitration of aromatic compounds by magnesium nitrate hexahydrate

By Hosseini-Sarvari, Mona and Tavakolian, Mina

From Journal of Chemical Research, (12), 722-724; 2008

3. Single Step



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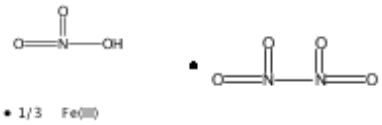
Overview

Steps/Stages

1.1 R:



S:Me_2CO, 150 h, rt

Notes

alternative prepn. shown, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

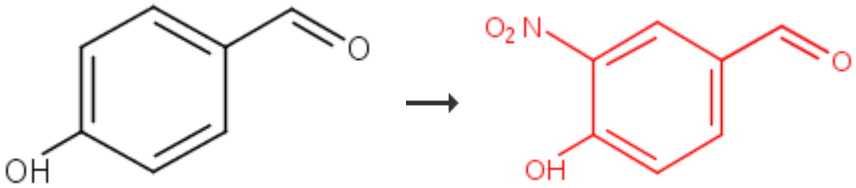
References

Selective mono-and dinitration of phenolic compounds by dinitrogen tetraoxide complexes of iron and copper nitrates as new nitration reagent

By Zhang, Ji-chang et al

From Henan Shifan Daxue Xuebao, Ziran Kexueban, 31(3), 61-65; 2003

4. Single Step



91%

Overview

Steps/Stages

1.1 R:HNO_3, S:MeCN, S:AcOH, 3 h, reflux

Notes

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

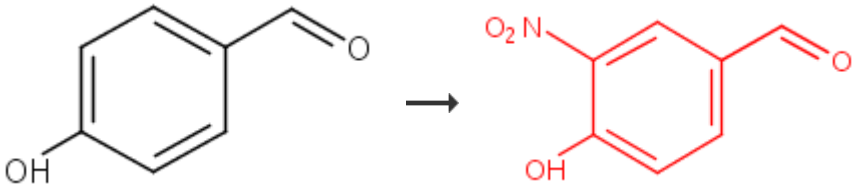
References

Selective photosensitization through an AND logic response: optimization of the pH and glutathione response of activatable photosensitizers

By Erbas-Cakmak, Sundus et al

From Chemical Communications (Cambridge, United Kingdom), 51(61), 12258-12261; 2015

5. Single Step



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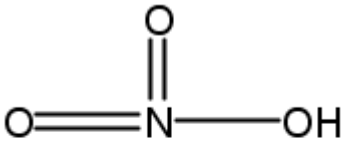
Overview

Steps/Stages

1.1 R:



• 1/3 Al

S:Me_2CO, 60 min, rt

Notes

regioselective, solid-supported reagent, Silica supported aluminum nitrate used, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

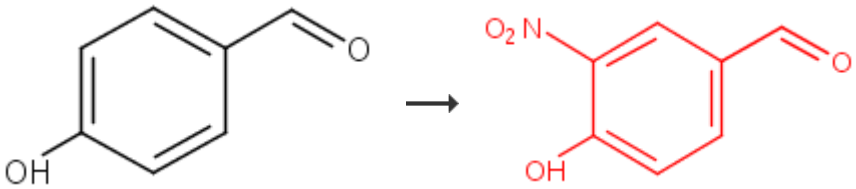
References

Regioselective Nitration of Phenols and Phenyl Ethers Using Aluminium Nitrate on Silica as a Nitrating System

By Patil, Mahadeo R. et al

From Letters in Organic Chemistry, 12(2), 129-135; 2015

6. Single Step



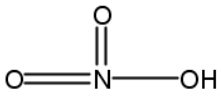
95%

Overview

Steps/Stages

Notes

1.1 R:



- 1/2 Mg

- 3 H_2O

C:H_2SO_4, C:Al_2O_3, S:H_2O, 3.5 h, 80°C

regioselective, green chemistry-solvent, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

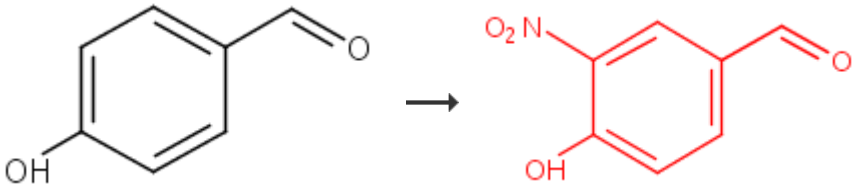
References

Nitration of aromatic compounds using alumina sulfuric acid (ASA) as a novel heterogeneous system and Mg(NO3)2.6H2O as nitrating agent in water

By Hosseini-Sarvari, M. et al

From Iranian Journal of Science and Technology, 34(A3), 215-225; 2010

7. Single Step



95%

Overview

Steps/Stages

1.1 C:Me_2BrS^+ •Br^-, C:Bu_4N^+ •$^-$ON=O, S:MeCN, 2 h, rt

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

Notes

regioselective, mechanism studied, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 2, Most stages in any one step: 2

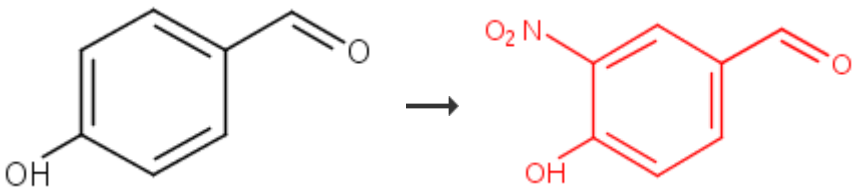
References

Bromodimethylsulfonium bromide/tetrabutylammonium nitrite, an efficient catalyst mixture for the nitration of phenols

By Akhlaghinia, Batool and Pourali, Alireza

From Turkish Journal of Chemistry, 34(5), 753-759; 2010

8. Single Step



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Overview

Steps/Stages

1.1 R:AcOH, R:HNO_3, S:MeCN, 3 h, reflux

Notes

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

References

Cascading of Molecular Logic Gates for Advanced Functions: A Self-Reporting, Activatable Photosensitizer

By Erbas-Cakmak, Sundus and Akkaya, Engin U.

From Angewandte Chemie, International Edition, 52(43), 11364-11368; 2013

Reaction Protocol

Procedure

1. Dissolve 4-hydroxybenzaldehyde (10 mmol) in 20 ml acetonitrile.
2. Reflux the reaction for 3 hours.

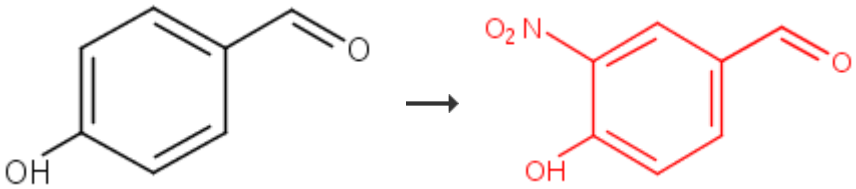
View more...

Available Experimental Data

^{1}H NMR, ^{13}C NMR

View with MethodsNow

9. Single Step



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Overview

Steps/Stages

1.1 R:HNO_3, S:MeCN, 3 h, reflux

Notes

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

References

Development of Luminescent Coelenterazine Derivatives Activatable by β-Galactosidase for Monitoring Dual Gene Expression

By Lindberg, Eric et al

From Chemistry - A European Journal, 19(44), 14970-14976; 2013

Reaction Protocol

Procedure

1. Reflux the solution of 4-hydroxybenzaldehyde (20.1 mmol) in acetonitrile (40 ml), with acetic acid (20 ml) and concentrate nitric acid (1.5 ml) for 3 hours.
2. Cool the solution to room temperature.

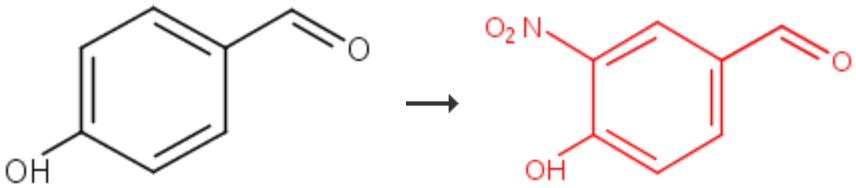
View more...

Available Experimental Data

State

View with MethodsNow

10. Single Step



97%

Overview

Steps/Stages

1.1 R:$NaNO_2$, R:SiO_2 (chlorinated), R:H_2O, S:CH_2Cl_2, 30 min, rt

Notes

silica chloride used, Reactants: 1, Reagents: 3, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Silica chloride/NaNO2 as a novel heterogeneous system for the nitration of phenols under mild conditions

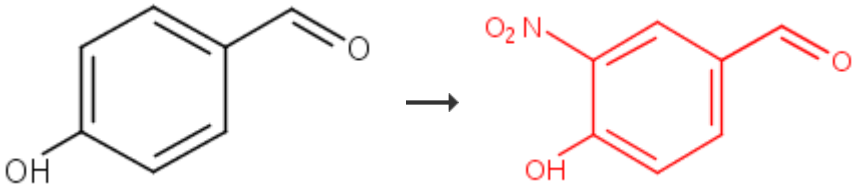
By Zolfigol, Mohammad Ali et al

From Phosphorus, Sulfur and Silicon and the Related Elements, 178(9), 2019-2025; 2003

Experimental Procedure

General/Typical Procedure: ***Mononitration of Phenol (1) with Silica Chloride (I), $NaNO_2$ (II), and Wet SiO_2: A Typical Procedure*** A suspension of compound **1** (0.188 g, 2 mmol), **I** (0.4 g), **II** (0.207 g, 3 mmol), and wet SiO_2 (50% *w/w,* 0.4 g) in CH_2Cl_2 (10 ml) was stirred magnetically at room temperature. The reaction was completed after 1 h and then filtered. The residue was washed with CH_2Cl_2 (2 x 10 ml). Anhydrous Na_2SO_4 (3 g) was added to the filtrate. After 15 min the resulting mixture was filtered. Dichloromethane was removed by water bath (35-40°C)* and simple distillation. The residue is a mixture of 2 and 4-nitrophenols. 4-Nitrophenol **(3)** is insoluble in n-pentane, 0.084 g, 31%. The n-pentane was evaporated by water bath (35-40°C),45 to give 2-nitrophenol **(4)**, 0.088 g, 32% (Table I, Scheme 2). **6i**, yield 97%. m.p. Found: 143-145°C; m.p. Reported: 140-142°C.

11. Single Step



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Overview

Steps/Stages

1.1 R:$Fe(NO_3)_3$, R:N_2O_4, S:Me_2CO

Notes

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

References

Dinitrogen tetroxide complexes of iron and copper nitrates as new reagents for selective mono- and dinitration of phenolic compounds

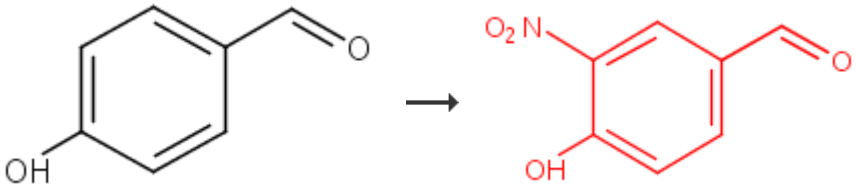
By Firouzabadi, H. et al

From Synthetic Communications, 27(19), 3301-3311; 1997

Experimental Procedure

General/Typical Procedure: **Mononitration of 4-Chlorophenol with $Fe(NO_3)_3.1.5\ N_2O_4$ as a Typical Procedure:** 4-Chlorophenol (0.257 g, 2 mmol) and $Fe(NO_3)_3.1.5\ N_2O_4$ (0.76 g, *2* mmol) were mixed together in acetone (4 mL) while being stirred vigorously at room temperature. The reaction was completed immediately. After column chromatography on Silica gel 4-chloro-2-nitrophenol was obtained as yellow needle crystals, 0.34 g,99%, Yield 100%.

12. Single Step



88%

Overview

Steps/Stages

Notes

1.1 R:Cl(O=)CC(=O)Cl, R:DMF, S:MeCN, -5°C

1.2 R:KNO_3, 2-3 min, 100°C, 2 bar

optimization study, optimized on reagent and methods (conventional and sonication), in-situ generated reagent (iminium salt) (stage 1), selective nitration, microwave irradiation (60 W), no solvent (stage 2), Reactants: 1, Reagents: 3, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Oxalyl chloride/DMF as an Efficient Reagent for Nitration of Aromatic Compounds and Nitro Decarboxylation of Cinnamic Acids in Presence of KNO3 or NaNO2 Under Conventional and Nonconventional Conditions

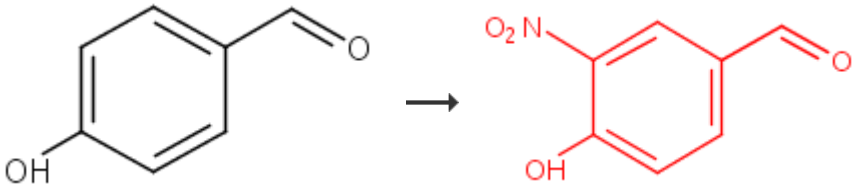
By Kumar, M. Satish et al

From Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry, 43(8), 977-983; 2013

Experimental Procedure

General/Typical Procedure: **Nitro Arenes and β-Nitro Styrenes Using $(COCl)_2$+DMF Iminium Salt Under Solvent-Free Conditions** Organic substrate, KNO_3 (or $NaNO_2$), $(COCl)_2$+DMF iminium salt and the resulting reaction mixture was heated in a controlled microwave synthesizer (Biotage Initiator + SP Wave model 0.200 W at 2.45 GHz, capped at 60 W during steady state) for 5 min (attains temperature 100 °C and 2 bar pressure) and progress of the reaction was monitored by TLC. After completion, the reaction mixture is further processed for the isolation of product as detailed in earlier section. **2-*Nitrophenol* 4-*OH*-3-*NO_2* *benzaldehyde*** Yield 88%. δ 11.01 (brs, 1H, -OH), 9.94 (s, 1H, -CHO), 8.63 (s, 1H, Ar-*H*), 8.14 (d, 1H, *J* = 3.5 Hz), 7.33 (d, 1H, *J* = 3.5 Hz, Ar-*H*); m/z = 167.

13. Single Step



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Overview

Steps/Stages

1.1 R:HNO_3, R:SiO_2, C:$Bi(NO_3)_3$, 6 min, rt

1.2 R:$Na_2S_2O_3$

Notes

regioselective, optimization study, no solvent, optimized on catalyst, alternate conventional method gave lower yield, microwave irradiation in stage 1, 140W used in stage 1, silica gel used in stage 1, Reactants: 1, Reagents: 3, Catalysts: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

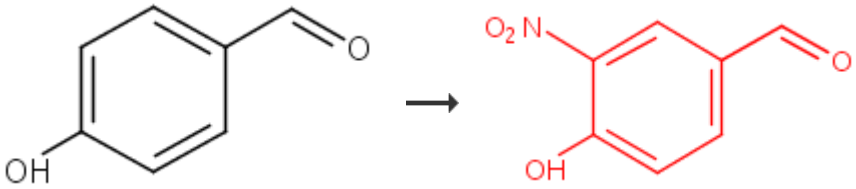
References

Mortar-pestle and microwave assisted regioselective nitration of aromatic compounds in presence of certain group V and VI metal salts under solvent free conditions

By Sariah, Sana et al

From International Journal of Organic Chemistry, 2(3), 233-247; 2012

14. Single Step



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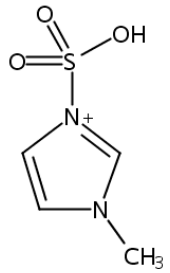
Overview

Steps/Stages

1.1 R:



- Cl -

R:$NaNO_2$, 25 min, rt

Notes

regioselective, green chemistry, green chemistry-reagent, green chemistry-waste reduction, ionic liquid used (reagent), mechanism studied, Reactants: 1, Reagents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

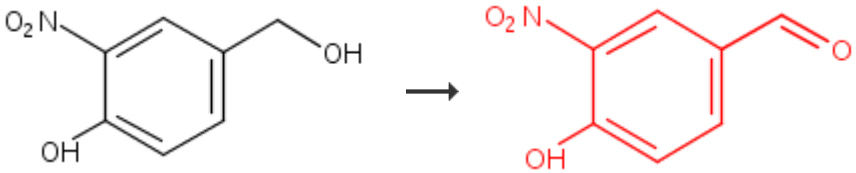
References

An efficient method for the nitration of phenols with NaNO2 in the presence of 3-methyl-1-sulfonic acid imidazolium chloride

By Khazaei, A. et al

From Scientia Iranica, Transaction C: Chemistry, Chemical Engineering, 17(1), 31-36; 2010

15. Single Step



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Overview

Steps/Stages

Notes

1.1 R:AcOH, C:1258980-63-0 immobilized on superparamagnetic iron oxid, C:$Cu(NO_3)_2$, C:10377-66-9, S:98-08-8, 2 h, 50°C

solid-supported catalyst, chemoselective, catalyst recyclable, >99% selectivity, [3-[4-(1-hydroxy-2,2,6,6-tetramethylpiperidin-4-yloxymethyl)-2,3-dihydro-[1,2,3]triazol-1-yl]propyl]phosphonic acid immobilized on superparamagnetic iron oxide nanoparticles with final TEMPO loading 0.50-0.93 mmol per gram used as catalyst, Reactants: 1, Reagents: 1, Catalysts: 3, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

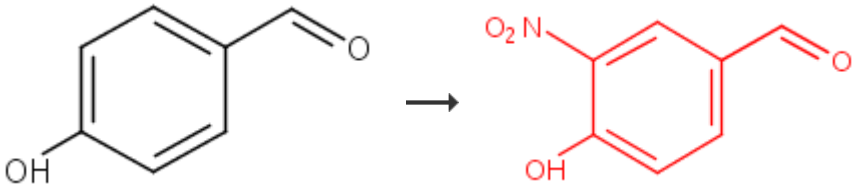
References

Simple Preparation and Application of TEMPO-Coated Fe3O4 Superparamagnetic Nanoparticles for Selective Oxidation of Alcohols

By Tucker-Schwartz, Alexander K. and Garrell, Robin L.

From Chemistry - A European Journal, 16(42), 12718-12726, S12718/1-S12718/31; 2010

16. Single Step



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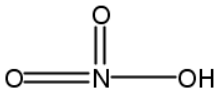
Overview

Steps/Stages

1.1 R:



- 3 H_2O

- 1/2 Zn

C:Cyanuric trichloride, S:MeCN, 70 min, rt

Notes

regioselective, optimization study, optimized on reagent, green chemistry-process simplification, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

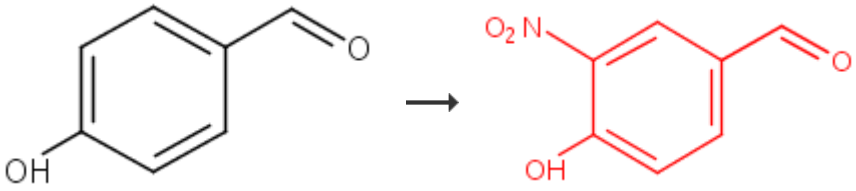
References

Zn(NO3)2·6H2O/2,4,6-trichloro-1,3,5-triazine (TCT) a mild and selective system for nitration of phenols

By Nemati, Firouzeh and Kiani, Hossein

From Chinese Chemical Letters, 21(4), 403-406; 2010

17. Single Step



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Overview

Steps/Stages

1.1 R:AcOH, R:HNO_3, S:H_2O, cooled; overnight

Notes

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

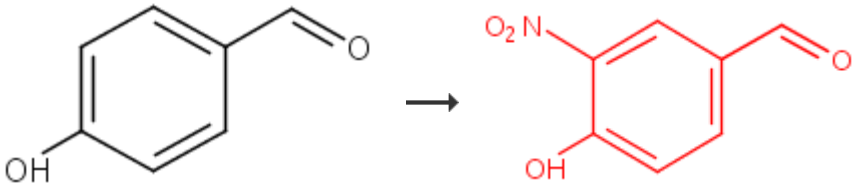
References

A coloured spin trap which works as a pH sensor

By Ionita, Petre

From South African Journal of Chemistry, 61, 123-126; 2008

18. Single Step



90%

Overview

Steps/Stages

1.1 R:N_2O_4 (polyethyleneglycol-supported), S:CH_2Cl_2, 15 min, rt

Notes

regioselective, solid-supported reagent, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

PEG-N2O4: An efficient nitrating agent for the selective mono- and dinitration of phenols under mild conditions

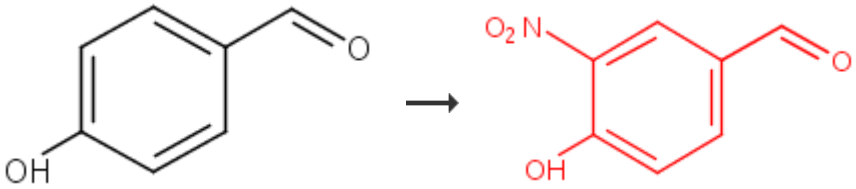
By Zolfigol, Mohammad Ali et al

From Synthetic Communications, 38(19), 3366-3374; 2008

Experimental Procedure

General/Typical Procedure: **Mononitration of 4-Substituted Phenols (5) with PEG-N_2O_4: A Typical Procedure** A solution of compound **5** (2 mmol) and PEG-N_2O_4 (0.8 g) in CH_2Cl_2 (8 mL) was magnetically stirred at room temperature for the time specified in Table 1. After completion of the reaction, the reaction mixture was passed through a short column of silica gel and washed with dichloromethane as eluent to separate PEG. The dichloromethane was removed by water bath (35-40 °C) and simple distillation to give the pure product. 6i, yield 90%.

19. Single Step



93%

Overview

Steps/Stages

1.1 R:HNO_3, S:MeCN, S:AcOH, 3 h, reflux

Notes

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

References

Synthesis and Fluorescence Sensing Properties of Calix[4]arenes Containing Fluorophores

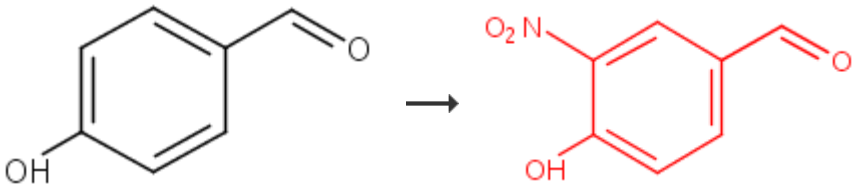
By Morakot, Nongnit et al

From Supramolecular Chemistry, 17(8), 655-659; 2005

Experimental Procedure

A mixture of *p*-hydroxybenzaldehyde (2.446 g, 20.0 mmol), acetic acid (20 mL), nitric acid (1.50 mL) and acetonitrile (40 mL) was refluxed for 3h. After cooling to room temperature, the solvent was evaporated off under reduced pressure. Ethyl acetate (30 mL) and water (30 mL) were added to the residue and the aqueous solution was extracted with ethyl acetate (2 X 50 mL). The combined organic layer was dried over anhydrous sodium sulfate and filtered. The filtrate was dried under reduced pressure. A brown solid **1a** (93% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ (in ppm) 10.05 (s, 1H, ArCHO), 8.68 (s, 1H, ArOH), 8.18 (d, *J* = 7, 1H, Ar), 7.37 (d, *J* = 8,1H, Ar), 7.35 (s, 1H, Ar).

20. Single Step



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Overview

Steps/Stages

Notes

1.1 R:HNO_3, C:12240-15-2, 160 s, rt

green chemistry-catalyst, microwave irradiation, no solvent, regioselective, optimization study, optimized on solvent, optimized on time, silica gel used, Reactants: 1, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Prussian Blue as an Ecofriendly Catalyst for Selective Nitration of Organic Compounds Under Conventional and Nonconventional Conditions

By Pasnoori, Srinivas et al

From Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry, 44(3), 364-370; 2014

Experimental Procedure

General/Typical Procedure: General Procedure for Microwave Assisted Synthesis of Nitro Arenes Under Solvent Free Conditions. 0.01 mol of organic substrate, PB (1 mmol), and a few drops of HNO_3 were taken in a previously cleaned 50 mL beaker. About 500 mg of silica gel were added to the contents and mixed thoroughly and placed in the laboratory microwave oven. Silica gel is added to adsorb liquid reactants and facilitate solvent-free conditions. After completion of the reaction, as confirmed by TLC, the reaction mixture is worked up as detailed in the earlier section to get pure product. Product: 4-OH-3-NO_2-benzaldehyde, Yield: 87%, pure product, Substrate: 4-OH-Benzaldehyde. Microwave: RT: 160 sec. δ 11.01 (brs, 1H, -OH), 9.94 (s, 1H, -CHO), 8.63 (s, 1H, Ar-H), 8.14 (d, 1H, *J* = 3.5 Hz), 7.33 (d, 1H, *J* = 3.5 Hz, Ar-H); m/z = 167.

Reaction Protocol

Procedure

1. Add 4-hydroxybenzaldehyde (0.01 mol), Prussian blue (1 mmol), and a few drops of HNO_3 to a clean 50 mL beaker.
2. Add silica gel (approximately 500 mg) to adsorb liquid reactants and facilitate solvent-free conditions.

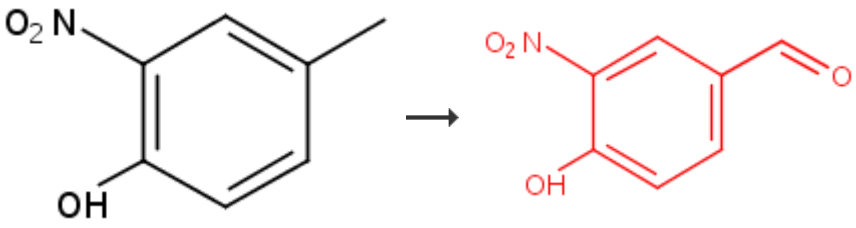
View more...

Available Experimental Data

^{1}H NMR, Mass Spec

View with MethodsNow

21. Single Step



87%

Overview

Steps/Stages **Notes**

1.1 R:NaOH, R:O_2, C:$Co(OAc)_2$, S:$(CH_2OH)_2$, 8 h, 80°C, 1 atm

green chemistry - catalyst, eco-friendly ligand-free transition-metal catalyzed selective aerobic oxidation, green chemistry - waste reduction, water is the only byproduct, green chemistry - reagent, atom-economy, Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Efficient Co(OAc)2-catalyzed aerobic oxidation of EWG-substituted 4-cresols to access 4-hydroxybenzaldehydes

By Jiang, Jian-An et al

From Tetrahedron Letters, 55(8), 1406-1411; 2014

Reaction Protocol

Procedure

1. Stir a mixture of cresol (1.0 mmol), $Co(OAc)_2 \cdot 4H_2O$ (0.01 mmol, 2.5 mg) and NaOH (2 equiv.) in EG (5 mL) with O_2 (1 atm) being bubbled, under 80 °C for 8 h.
2. Successively add hydrochloric acid (10 mL, 2%) and MTBE (10 mL) to the reaction mixture at room temperature.

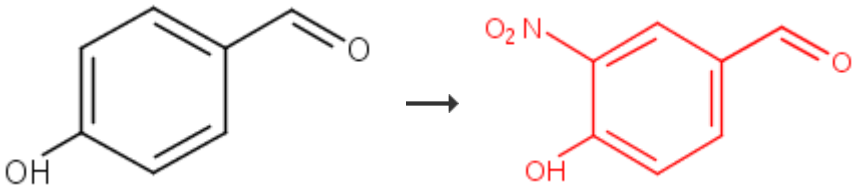
View more...

Available Experimental Data

^{1}H NMR, ^{13}C NMR, HRMS, MP, State

View with MethodsNow

22. Single Step

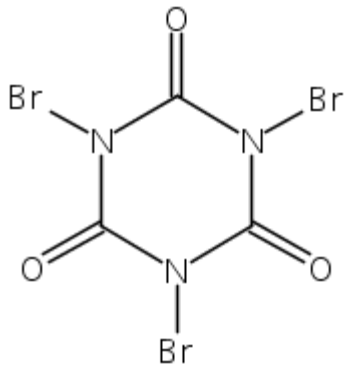


91%

Overview

Steps/Stages **Notes**

1.1 R:



green chem., alternative reaction conditions gave lower yield, silica gel used (wet), Reactants: 1, Reagents: 4, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

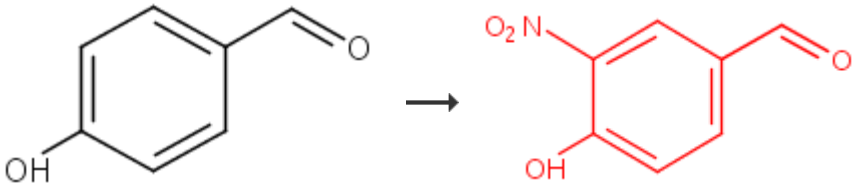
Tribromoisocyanuric acid/NaNO2: a new reagent for mononitration of phenols under mild and heterogeneous conditions

By Niknam, Khodabakhsh et al

From South African Journal of Chemistry, 60, 109-112; 2007

R:$NaNO_2$, R:SiO_2, R:H_2O, S:CH_2Cl_2, 60 min, rt

23. Single Step



90%

Overview

Steps/Stages

1.1 R:$Fe(NO_3)_3 \cdot 9H_2O$, S:CH_2Cl_2, 20 min, rt

Notes

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

References

Mild and selective nitration of phenols by zeofen

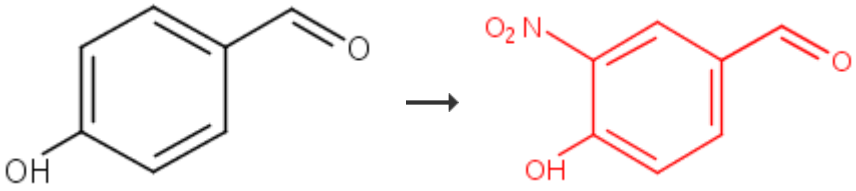
By Bigdeli, Mohammad A. et al

From Synthetic Communications, 37(13), 2225-2230; 2007

Experimental Procedure

General/Typical Procedure: **Nitration of Phenols with Zeofen: Typical Procedure** 4-Chloro phenol (0.12 g, 1 mmol) and zeofen (1-1.5 eq.) in 3 mL of dichloromethane were magnetically stirred at room temperature. After the completion of the reaction, the reaction mixture was filtered (the progress of the reaction was monitored by TLC). The residue was washed with CH_2Cl_2 (2 x 5 mL) and dried over anhydrous sodium sulfate. The solvent was removed under vacuum. The crude product was purified by silica-gel dry flash chromatography using petroleum ether-ethyl acetate (98:2) as eluent. The yield was 0.15 g (88%). ***Table 1***, Entry 8, yield 90%.

24. Single Step

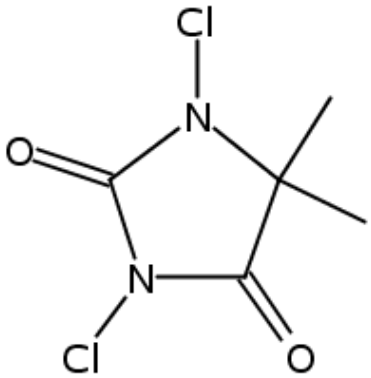


90%

Overview

Steps/Stages

1.1 R:



R:$NaNO_2$, R:H_2O, S:$Me(CH_2)_4Me$, 45 min, rt

Notes

regioselective, green chem.-reagent, optimization study, optimized on reagent, water/reagent on SiO2 used, Reactants: 1, Reagents: 3, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

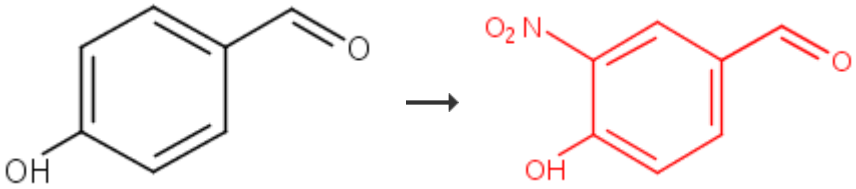
References

1,3-Dihalo-5,5-dimethylhydantoin or citric acid/NaNO2 as a heterogeneous system for the selective mononitration of phenols under mild conditions

By Zolfigol, Mohammad A. et al

From Mendeleev Communications, (1), 41-42; 2006

25. Single Step



82%

Overview

Steps/Stages

1.1 R:HNO_3, S:H_2O, S:AcOH, heated; < 110°C

Notes

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

References

Some new energetic benzaldoximes

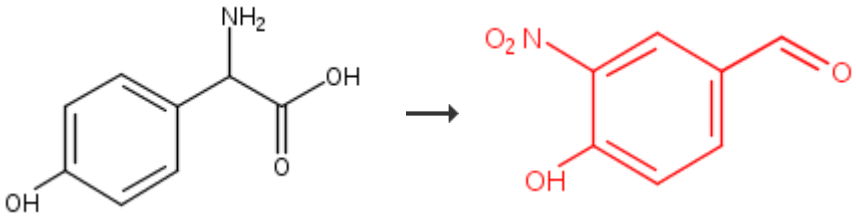
By Kunduraci, Melike et al

From Journal of Thermal Analysis and Calorimetry, 112(3), 1587-1599; 2013

Experimental Procedure

Synthesis of 3-nitro-4-hydroxy benzaldehyde. It was synthesized according to the method described in the literature. 5 g of 4-hydroxy benzaldehyde was dissolved in 25 mL of CH_3COOH at hydrothermal conditions and the solution was heated. 10 mL of HNO_3 (63 %) was added to this solution and the mixture was stirred while keeping the temperature below 110 °C. Then, the solution was poured into 250 mL ice-water mixture, filtered, and dried in the oven at 60 °C. Yield 82 %. IR Data (cm^{-1}) ν_{O-H}= 3228 $\nu_{C=O}$= 1683 $\nu_{C=C}$= 1610 $\nu_{N=O}$= 1329 $\nu_{C-H(Ar)}$= 3092-3063 $\nu_{C-H(Ald)}$= 2871 $\delta_{C-H(Ar)}$= 740.

26. Single Step



85%

Overview

Steps/Stages

1.1 R:HNO_3, S:H_2O, 12 h, 60°C; 60°C → 0°C

Notes

regioselective, product depends on reaction conditions, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

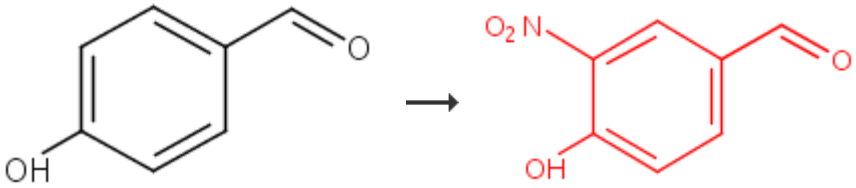
References

New one-pot synthesis of 4-hydroxybenzaldehyde derivatives and picric acid from 4-hydroxyphenylglycine with HNO3/H2O

By Shin, Young-Gyun and Yoon, Sung-Hwa

From Bulletin of the Korean Chemical Society, 30(11), 2819-2822; 2009

27. Single Step



85%

Overview

Steps/Stages

Notes

1.1 R:HNO_3, C:13530-50-2, S:H_2O, rt; 30 min, 60°C

regioselective, green chem.-catalyst, green chem.-process simplification, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

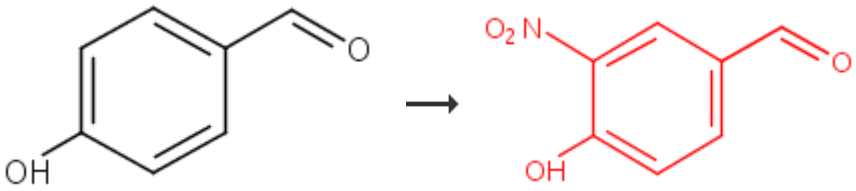
References

Al(H2PO4)3. An efficient catalyst for nitration of organic compounds with nitric acid

By Bharadwaj, Saitanya K. et al

From Catalysis Communications, 9(5), 919-923; 2008

28. Single Step



85%

Overview

Steps/Stages

Notes

1.1 R:HNO_3, C:13765-94-1, S:PhMe, S:H_2O, 30 min, 60°C

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

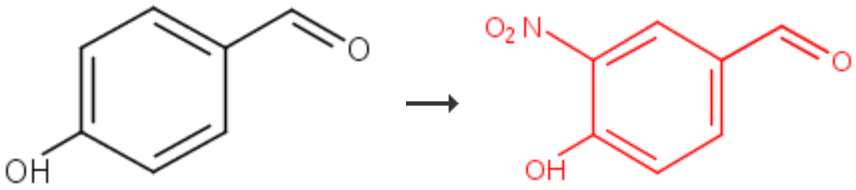
References

Acid phosphate-impregnated titania-catalyzed nitration of aromatic compounds with nitric acid

By Bharadwaj, Saitanya K. et al

From Applied Catalysis, A: General, 343(1-2), 62-67; 2008

29. Single Step



89%

Overview

Steps/Stages

Notes

1.1 R:HNO_3, S:AcOH, 30 min, 50-55°C

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

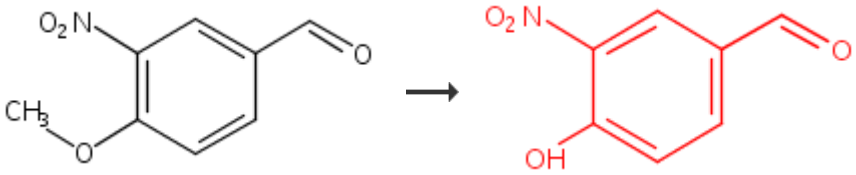
References

New method for the synthesis of 4-hydroxy-3-iodo-5-nitrobenzonitrile

By Zhao, Hai-shuang et al

From Huaxue Shiji, 25(4), 237-238, 240; 2003

30. Single Step



89%

Overview

Steps/Stages

Notes

1.1 R:Me_3SiI, S:$CHCl_3$

in-situ generated reagent, alternative solvent CCl4, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

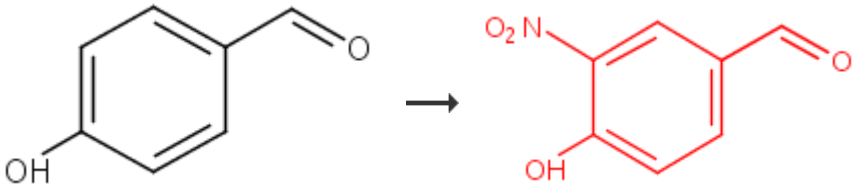
References

Demethylation of some aryl methyl ethers and selective demethylation of some pyrones by the use of iodotrimethylsilane

By Younis, Y. M. H.

From International Journal of Chemistry (Calcutta, India), 11(2), 75-85; 2001

31. Single Step



90%

Overview

Steps/Stages

Notes

1.1 R:N_2O_4 (reaction product with chromyl chloride), S:Me_2CO

no dinitration seen, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Efficient and selective mono and dinitration of phenols with Cr(NO3)3.2N2O4 as a new nitrating agent

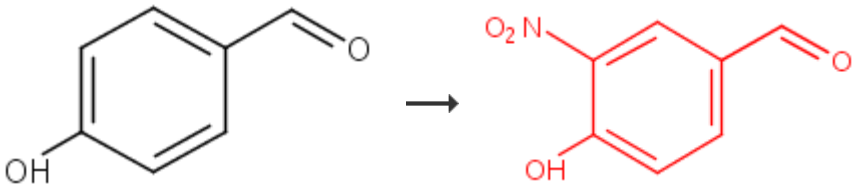
By Iranpoor, Nasser et al

From Synthetic Communications, 28(15), 2773-2781; 1998

Experimental Procedure

General/Typical Procedure: **General Procedure for Mono or Dinitration of 4-Substituted Phenols:** To a solution of the phenolic compound (2 mmol) in appropriate solvent (4 ml), was added $Cr(NO_3)_{3.bul.}2N_2O_4$ (the molar ratio of the reagent to the substrate was optimized on the basis of the required conditions for mono or dinitration reactions Table 3) the mixture was stirred vigorously at room temperature or under reflux conditions. The progress of the reaction was monitored by TLC. The reaction mixture was presorbed on silica gel (5 g) and the resulting mixture was applied on a short column on silica gel and eluted with petroleum ether.acetone (9:1) and petroleum ether:EtOAc (3:1) for the separation and purification of mono and dinitrated products respectively. yield 90%.

32. Single Step



95%

Overview

Steps/Stages

1.1 R:$Fe(NO_3)_3$, S:PhMe

Notes

montmorillonite clay supported iron nitrate, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

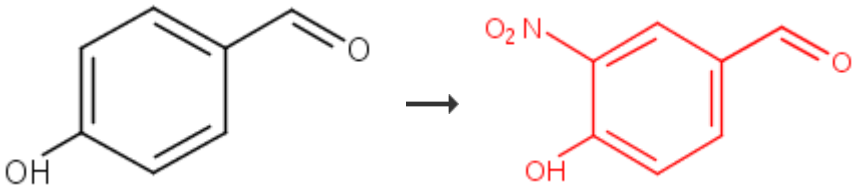
References

Study of the reactivity of metal nitrates adsorbed on montmorillonite

By Bekassy, Sandor and Cseri, Tivadar

From Magyar Kemiai Folyoirat, 97(8), 339-43; 1991

33. Single Step

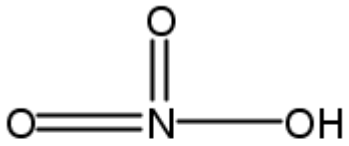


81%

Overview

Steps/Stages

1.1 R:



• 1/3 Al

R:Ac_2O, S:AcOH, 2 h, 30-40°C

Notes

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

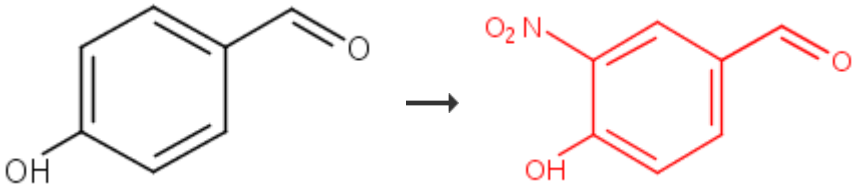
References

Synthesis, characterization, and antimicrobial activity of new series of benzoxazole derivatives

By Balaswamy, G. et al

From International Journal of Chemical Sciences, 10(4), 1830-1836; 2012

34. Single Step



85%

Overview

Steps/Stages

1.1 R:$Ce(NH_4)_2(NO_3)_6$, 2-4 min, rt; 8 min, heated

Notes

reaction at room temp. gives decreased yield over longer time, microwave irradiation, no solvent, regioselective, solid state, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

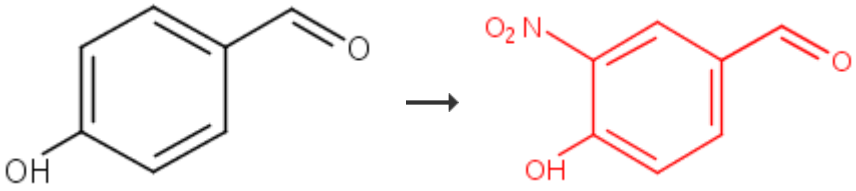
References

Solid-state regioselective nitration of activated hydroxyaromatics and hydroxycoumarins with cerium(IV) ammonium nitrate

By Ganguly, Nemai C. et al

From Journal of Chemical Research, (11), 733-735; 2005

35. Single Step



85%

Overview

Steps/Stages

1.1 R:HNO_3, S:CH_2Cl_2, 1 min, rt → 85°C

Notes

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

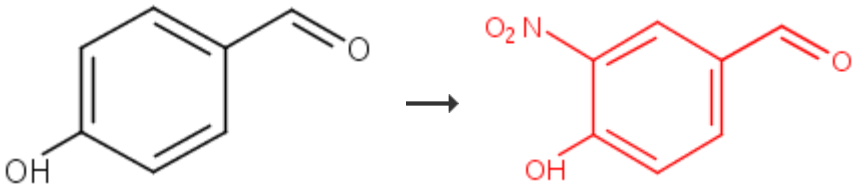
References

Microwave assisted synthesis of an unusual dinitro phytochemical

By Bose, Ajay K. et al

From Tetrahedron Letters, 45(6), 1179-1181; 2004

36. Single Step



78%

Overview

Steps/Stages

1.1 R:$NaNO_3$, R:Ortho-Gynol, R:HCl, S:H_2O, 60 min, 40°C

1.2 R:H_2O, R:CH_2Cl_2

Notes

regioselective, agitation (300 rpm), Reactants: 1, Reagents: 5, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Regioselective nitration of phenols by NaNO3 in microemulsion

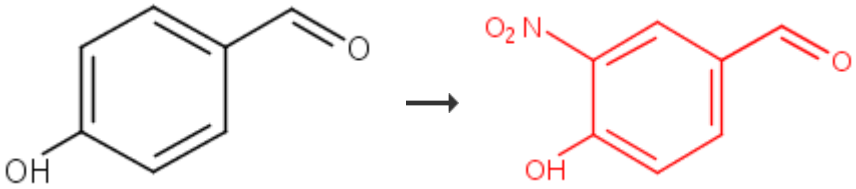
By Jiang, Jian-Zhong et al

From Journal of Dispersion Science and Technology, 32(1), 125-127; 2011

Experimental Procedure

General/Typical Procedure: 2.2. Reaction in Microemulsions: The experiments were carried out by adding the relevant weight ratio of surfactant, *n*-heptane, *n*-butanol, and distilled water into a 50mL flask. An amount of 1.6 mmol $NaNO_3$ and 0.8 mmol phenol were then added to the flask and the mixture was stirred at 40°C until an optically clear single-phase solution was formed. 0.8mL dilute hydrochloric acid (10 mol=L) were then added to the system. The reaction was monitored by gas chromatography (GC) and quenched by water and CH_2Cl_2. The oil phase was collected and dried, and the products were purified by column chromatography over silica gel. Products in the resulting mixture were analyzed by gas chromatography-mass spectroscopy (GC=MS). Product 7, yield 78%.

37. Single Step

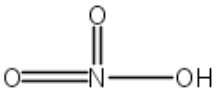


80%

Overview

Steps/Stages

1.1 R:



- 1/3 Bi(III)

- 5/3 H_2O

S:Me_2CO, 6 h, rt

Notes

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

References

Highly efficient nitration of phenolic compounds in solid phase or solution using Bi(NO3)3·5H2O as nitrating reagent

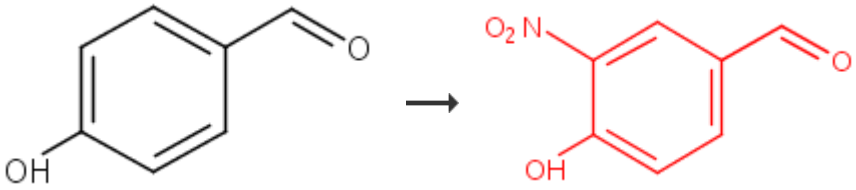
By Sun, Hong-Bin et al

From Journal of Organic Chemistry, 70(22), 9071-9073; 2005

Experimental Procedure

General/Typical Procedure: **(2) In Acetone Solution.** To a solid mixture of phenol (1.0 mmol) and $Bi(NO_3)_3.5H_2O$ (1.0 mmol) was added acetone (5.0 mL), the resulting mixture was then stirred at ambient temperature for ca. 3-4 min. The insoluble materials were filtered out immediately and washed by CH_2Cl_2 (10 mL), and the filtrate was concentrated. The nitrated products were isolated as described above to give 2-nitrophenol and 4-nitrophenol in 46% (64.0 mg, 0.46 mmol) and 47% (65.3 mg, 0.47 mmol) yield, respectively. **4-Hydroxy-3-nitro-benzaldehyde** (Table 2, entry 10): 167 (M^+, 71), 166 (100), 120 (27), 109 (3), 92 (20), 81 (11), 63 (47), 53 (24), 39 (28), 30 (14).

38. Single Step



93%

Overview

Steps/Stages

Notes

1.1

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

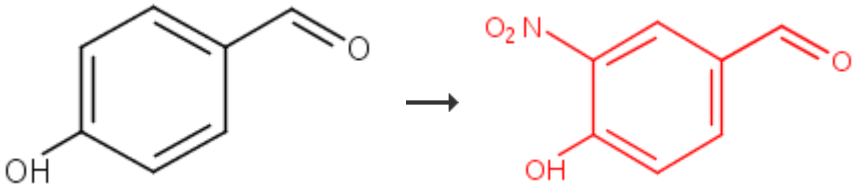
References

Nitration of phenols by clay-supported ferric nitrate

By Cornelis, A. et al

From Bulletin des Societes Chimiques Belges, 93(11), 961-72; 1984

39. Single Step



75%

Overview

Steps/Stages

1.1 R:HNO_3, C:V_2O_5, S:H_2O, 100 s, 150°C

1.2 R:$NaHCO_3$, S:H_2O

Notes

regioselective, microwave irradiation (140W), silica gel used, thermal, alternative reaction conditions shown, Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

Vanadium pentoxide as a catalyst for regioselective nitration of organic compounds under conventional and nonconventional conditions

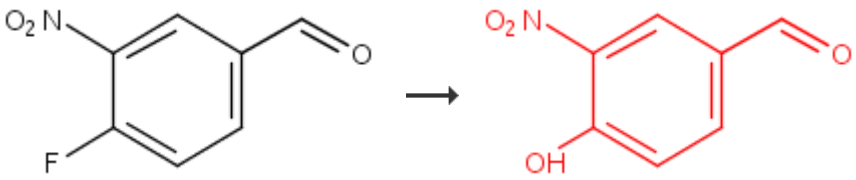
By Venkatesham, N. et al

From Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry, 44(7), 921-926; 2014

Experimental Procedure

General/Typical Procedure: **Typical Experimental Procedure for Microwave-Assisted Nitration (MWANR) of Organic Compounds** Themicrowave (MW) reactor usedwas of CEM make,which was equipped with temperature, pressure, and MW power control units. An oven-dried MW vial was charged with a mixture containing aromatic compound, V_2O_5 (9 mg, 0.005 mmol) and 69% HNO_3 (0.063 mL, 1 mmol) and silica gel slurry, and irradiated in a MW(power input 140 W) at 150°C for few minutes. After completion of the reaction, as ascertained by TLC, the reactionmixture was treated with sodium bicarbonate; the organic layer was diluted with dichloromethane (DCM) and separated from aqueous layer. The crude product mixture was purified with ethyl acetate DCM mixture. The purity was checked with TLC. The products were identified by characteristic spectroscopic data. ***4-OH 3-NO_2 Benzaldehyde.*** 11.28 δ (s 1H, OH) 10.34 δ (s 1H, CHO) 7.26 δ (d6, 1H, dd, *J* = 7.5 Hz) 7.64 δ (d 1H, d *J* = 7.5 Hz) 8.38 δ (s 1H); m/z = 167.

40. Single Step

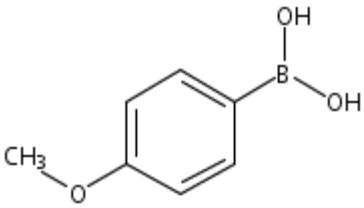


75%

Overview

Steps/Stages

1.1 R:



R:Cs_2CO_3, R:$Bu_4N^+ \cdot Br^-$, C:161265-03-8, C:$Pd(OAc)_2$, S:$(CH_2OMe)_2$, 70°C

Notes

Suzuki-Miyaura reaction condition, Reactants: 1, Reagents: 3, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

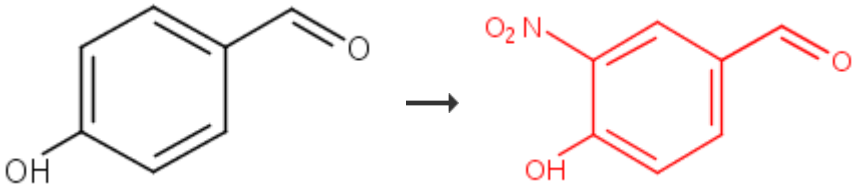
References

Unexpected palladium catalyzed O-arylation occurring in 4-(4-fluoro-3-nitrophenyl)-1,2-dimethyl-5-nitro-1H-imidazole series

By Zink, Laura et al

From Tetrahedron Letters, 53(40), 5393-5397; 2012

41. Single Step

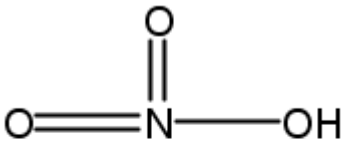


78%

Overview

Steps/Stages

1.1 R:



• 1/2 Ca

R:AcOH, 1 min, heated

Notes

green chem., microwave irradn. (400W), 80% aqueous acetic acid can also be used, Reactants: 1, Reagents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

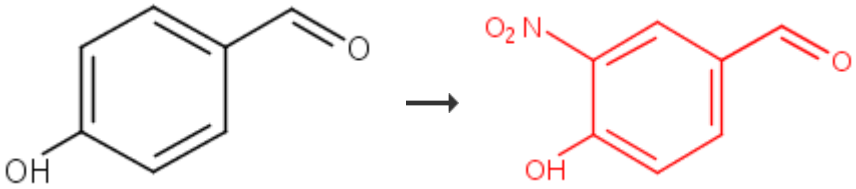
References

Microwave promoted rapid nitration of phenolic compounds with calcium nitrate

By Bose, Ajay K. et al

From Tetrahedron Letters, 47(12), 1885-1888; 2006

42. Single Step



80%

Overview

Steps/Stages

1.1 R:HNO_3, C:$ZnCl_2$, S:AcOEt, 30 min, 30°C

Notes

chemoselective, regioselective, ultrasound, silent conditions gave lower yield and reaction rate, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

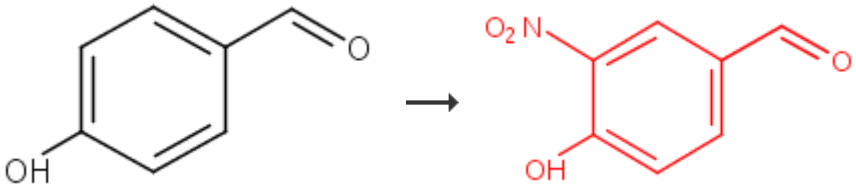
References

An efficient and facile nitration of phenols with nitric acid/zinc chloride under ultrasonic conditions

By Kamal, Ahmed et al

From Ultrasonics Sonochemistry, 11(6), 455-457; 2004

43. Single Step



78%

Overview

Steps/Stages

1.1 R:Isocyanuric chloride, R:$NaNO_2$, C:SiO_2, S:CH_2Cl_2, 20 min, rt

Notes

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

References

Trichloroisocyanuric acid/NaNO2 as a novel heterogeneous system for the selective mononitration of phenols under mild conditions

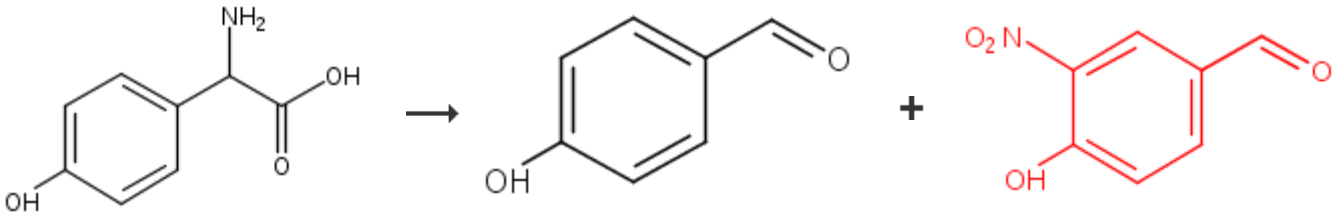
By Zolfigol, Mohammad Ali et al

From Synlett, (2), 191-194; 2003

Experimental Procedure

General/Typical Procedure: **Mononitration of 4-Chlorophenol (5b) with trichloroisocyanuric acid (I), $NaNO_2$ (II) and wet SiO_2: A Typical Procedure** A suspension of compound **5b** (0.257 g, 2 mmol), **I** (0.464 g, 2 mmol), wet SiO_2 (50% w/w, 0.4 g) and **II** (0.138 g, 2 mmol) in dichloromethane (10 mL) was stirred at room temperature for 15 min (the progress of the reaction was monitored by TLC) and then filtered. Anhydrous Na_2SO_4 (3 g) was added to the filtrate. After 15 min the resulting mixture was also filtered. Dichloromethane was removed by water bath (35-40 °C) under simple distillation to give (**6b**). **6i**, yield 78%. Mp: Found 143-145 °C, Reported 140-42[8c] °C.

44. Single Step



93% **7%**

Overview

Steps/Stages

1.1 R:HNO_3, S:H_2O, 1 h, rt; rt → 0°C

Notes

regioselective, alternative preparation decreased yield, alternatively reaction carried out for twenty-four hours decreased yield, alternatively reaction carried out using 50% concentrated nitric acid for twelve hours decreased yield, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

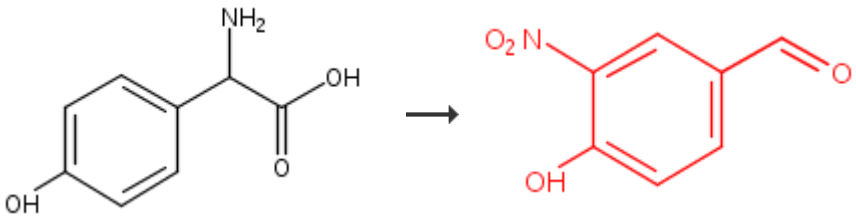
References

New one-pot synthesis of 4-hydroxybenzaldehyde derivatives and picric acid from 4-hydroxyphenylglycine with HNO3/H2O

By Shin, Young-Gyun and Yoon, Sung-Hwa

From Bulletin of the Korean Chemical Society, 30(11), 2819-2822; 2009

45. Single Step



70%

Overview

Steps/Stages **Notes**

1.1 R:HNO_3, S:H_2O, 12 h, 60°C

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

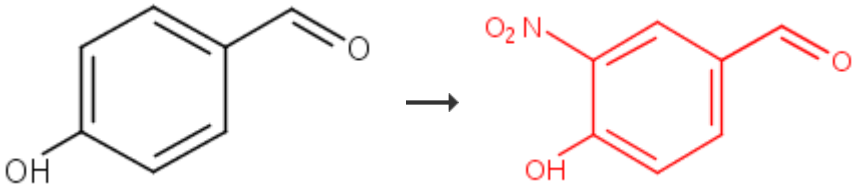
References

Method for preparing benzaldehyde derivative from phenylglycine compound

By Yoon, Seong Hwa et al

From Repub. Korea, 892233, 09 Apr 2009

46. Single Step

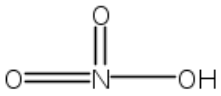


72%

Overview

Steps/Stages

1.1 R:



- 1/2 Ni(II)

- 3 H_2O

C:*p*-$MeC_6H_4SO_3H$, S:Me_2CO, 60 min, rt

Notes

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

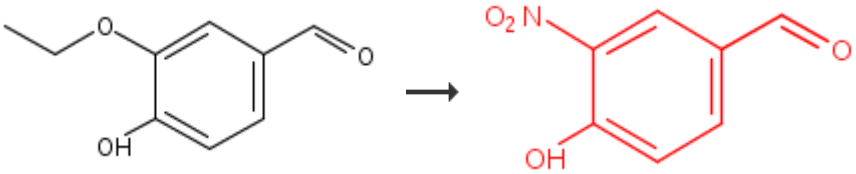
References

p-Toluenesulfonic acid-catalyzed regiospecific nitration of phenols with metal nitrates

By Anuradha, V. et al

From Tetrahedron Letters, 47(28), 4933-4935; 2006

47. Single Step



61%

Overview

Steps/Stages

Notes

1.1 R:HNO_3, S:AcOH, 20°C; 1 h, rt

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

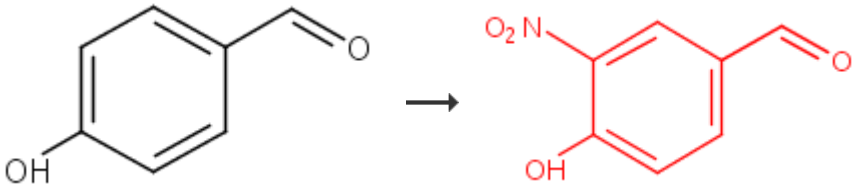
References

Investigation of ferulaic acid and its analogs: synthesis and scavenging free radicals

By Huang, Hua-yong et al

From Zhongguo Xinyao Zazhi, 15(6), 454-457; 2006

48. Single Step



61%

Overview

Steps/Stages

1.1 R:HNO_3 •NO_2, S:AcOH, < 0°C; 2 h, rt

Notes

fuming nitric acid used, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Synthesis and absorption spectra of poly(3-(phenylenevinyl)thiophene)s with conjugated side chains

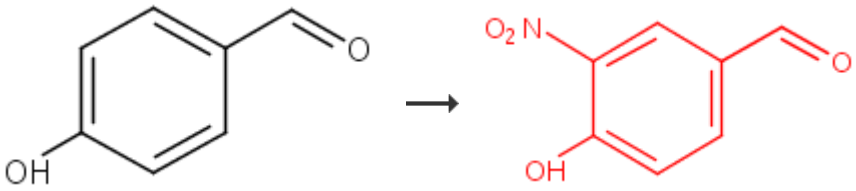
By Hou, Jianhui et al

From Macromolecules, 39(2), 594-603; 2006

Experimental Procedure

4-Hydroxy-3-nitrobenzaldehyde, 8. 4-Hydroxybenzaldehyde (0.2 mol, 24.4 g) was put into a flask, and glacial acetic acid (50 mL) was added. Under the ice-salt bath, fuming nitric acid (0.2 mol) was dropped into the flask below 0 °C. After the addition of nitric acid, the ice-salt bath was removed, and the reactants were stirred for 2 h at room temperature. Then, the mixture were poured into cracked ice. The solid was filtered and washed by a little icewater. After being recrystallized from alcohol, 20.1 g (0.12 mmol, yield 61%) of 4-hydroxy-3-nitrobenzaldehyde was obtained. GCMS: *m/z* = 167. ^{1}H NMR (δ, $CDCl_3$): 9.87 (s, 1H), 8.75 (s, 1H), 8.03 (d, 1H), 7.52 (d, 1H), 4.90 (s, 1H). Calculated for $C_7H_5NO_4$: C = 50.31; H = 3.02; N = 8.38; found: C = 50.25; H = 3.12; N= 8.29.

49. Single Step



Overview

Steps/Stages

1.1 R:HNO_3, S:AcOH

Notes

Claisen Smith reaction, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

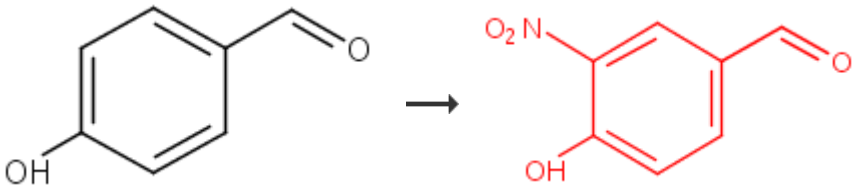
References

Design, synthesis and nonlinear optical properties of (E)-1-(4-substituted)-3-(4-hydroxy-3-nitrophenyl) prop-2-en-1-one compounds

By Saha, Amrita et al

From Chemical Physics Letters, 653, 184-189; 2016

50. Single Step



59%

Overview

Steps/Stages

1.1 R:KNO_3

Notes

reaction run in polyphosphoric acid, reaction temp. crit. to yield, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

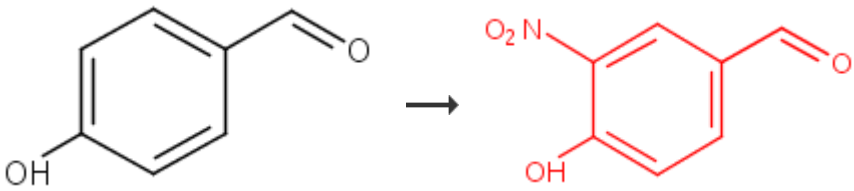
References

Nitration of some substituted aromatic compounds with potassium nitrate in polyphosphoric acid

By Iqbal, Rashid et al

From Journal of the Chemical Society of Pakistan, 19(2), 141-144; 1997

51. Single Step



60%

Overview

Steps/Stages

1.1 R:HNO_3

Notes

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

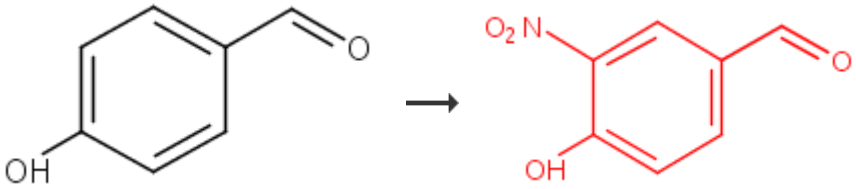
References

Synthesis and biological screening of 5-(nitroaryl)-substituted oxa/thiadiazoles

By Andotra, C. S. et al

From Journal of the Indian Chemical Society, 69(3), 169-70; 1992

52. Single Step



Overview

Steps/Stages

1.1

Notes

Go to Science of Synthesis, a critically reviewed reference work of synthetic methodology, for more information., Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

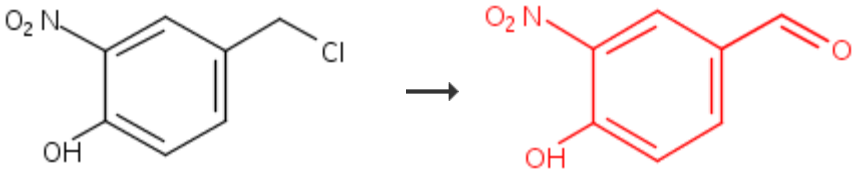
References

Nitroarenes

By Aitken, K. M. and Aitken, R. A.

From Science of Synthesis, 31b, 1183-1320; 2007

53. Single Step



70%

Overview

Steps/Stages

Notes

1.1 R:Hexamethylentetramine, S:CCl_4, S:AcOH

Classification: Oxidation; C-Amination; Hydrolysis; # Conditions: hexamine CCl4; Rf; AcOH; Rf; # Comments: Sommelet reaction, Reactants: 1, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

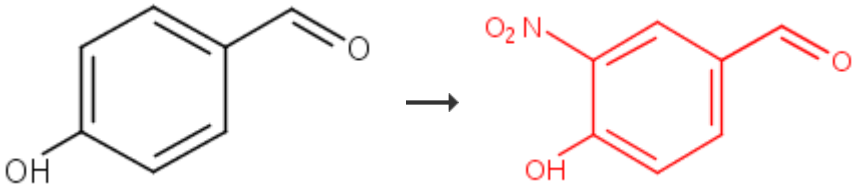
References

Sommelet reaction. III. The choice of solvent and the effect of substituents

By Angyal, S. J. et al

From Journal of the Chemical Society, , 2141-5; 1950

54. Single Step



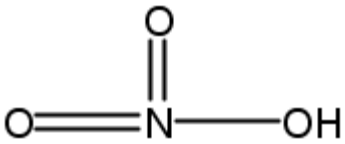
41%

Overview

Steps/Stages

Notes

1.1 R:



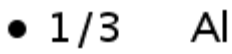
regioselective, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Process for nitration of phenols with aluminum nitrate

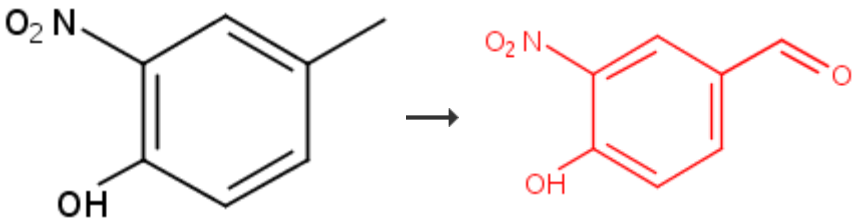
By Gou, Shaohua and Hu, Dahua

From Faming Zhuanli Shenqing, 1736976, 22 Feb 2006



S:EtOH, 9 h, reflux

55. Single Step



Overview

Steps/Stages

1.1 C:DDQ

Notes

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

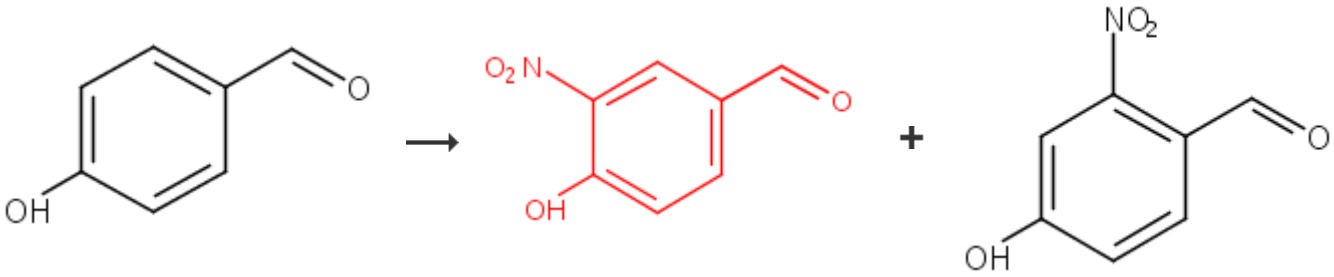
References

A convenient synthesis of p-hydroxybenzaldehydes

By Bird, C. W. and Chauhan, Y. P. S.

From Organic Preparations and Procedures International, 12(3-4), 201-2; 1980

56. Single Step



77% **17%**

Overview

Steps/Stages

1.1 R:NO_2

Notes

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

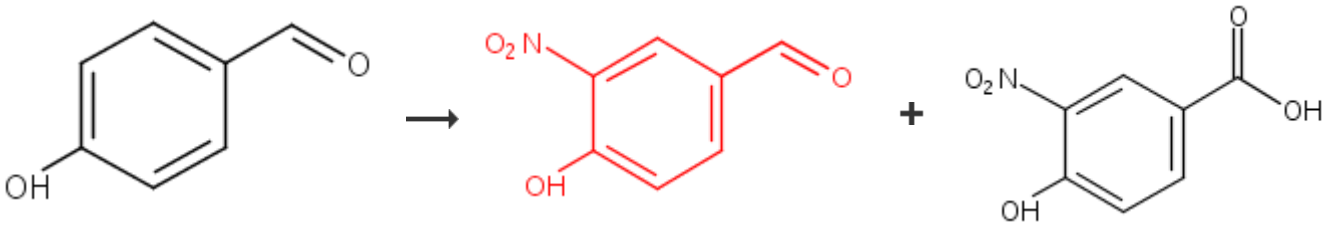
References

Gas/Solid Reactions with Nitrogen Dioxide

By Kaupp, Gerd and Schmeyers, Jens

From Journal of Organic Chemistry, 60(17), 5494-503; 1995

57. Single Step



Overview

Steps/Stages

Notes

1.1 R:HNO_3, C:H_3PO_4, S:H_2O, 30 min, rt

green chemistry-catalyst, regioselective, solid-supported catalyst, mixture yield, 68%, montmorillonite clay support, catalyst prepared and used, reusable catalyst, Reactants: 1, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

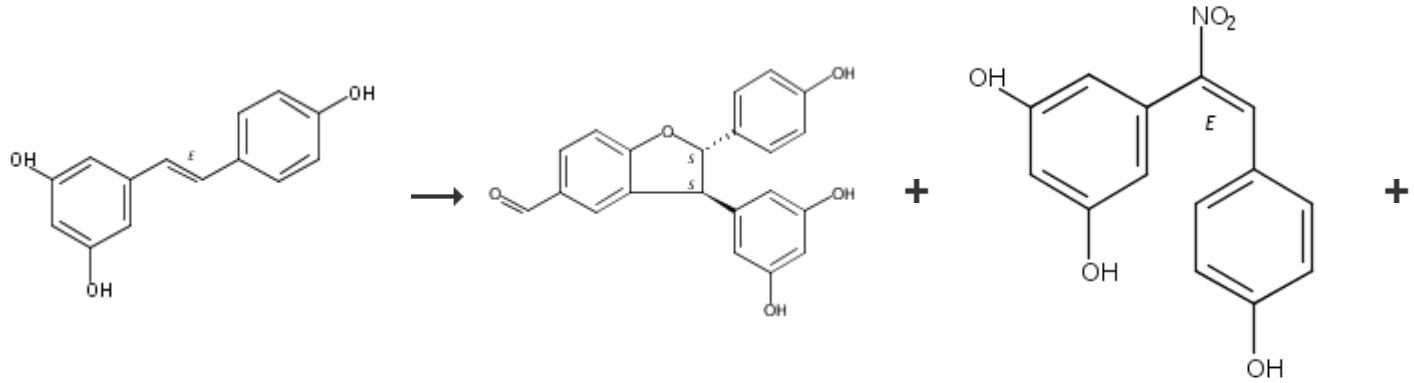
References

Phosphoric acid modified montmorillonite clay: A new heterogeneous catalyst for nitration of arenes

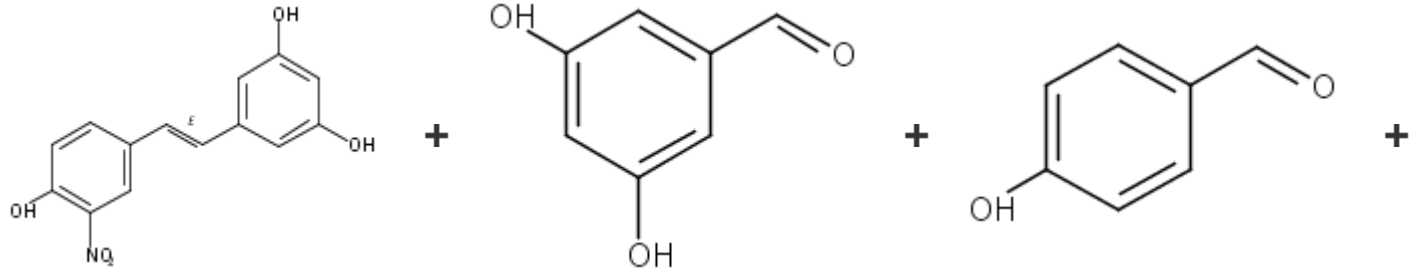
By Bharadwaj, Saitanya K. et al

From Catalysis Communications, 57, 124-128; 2014

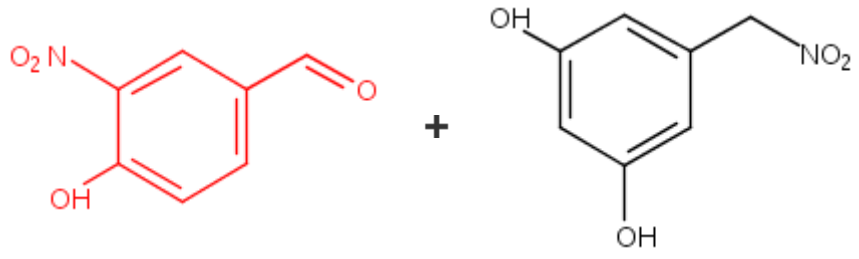
58. Single Step



2% **4%**



1% **4%**



1%

Overview

Steps/Stages **Notes**

1.1 R:$NaNO_2$, S:H_2O, S:MeOH, 3 h, rt, pH 3

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

References

Acid-Promoted Reaction of the Stilbene Antioxidant Resveratrol with Nitrite Ions: Mild Phenolic Oxidation at the 4'-Hydroxystiryl Sector Triggering Nitration, Dimerization, and Aldehyde-Forming Routes

By Panzella, Lucia et al

From Journal of Organic Chemistry, 71(11), 4246-4254; 2006

Experimental Procedure

Reaction of 1a with $NaNO_2$. General Procedure. To a solution of **1a** (10 mg, 44 Mmol) in methanol (0.5 mL) was added 0.1 M phosphate buffer (pH 3.0) (44 mL) followed by $NaNO_2$ (15 mg, 0.22 mmol), and the mixture was taken under vigorous stirring at room temperature. After 3 h, at complete consumption of the substrate (HPLC analysis, eluant A), the mixture was extracted with ethyl acetate (3 x 30 mL) and the combined organic layers were dried over Na_2SO_4 and taken to dryness. The residue was dissolved in methanol and analyzed by HPLC (eluant A), TLC, and LC/MS. In other experiments, the reaction of **1a** was run (i) as above with **1a** at 3 x 10^{-6} or 25 x 10^{-6} M concentration, with 0.2 x 10^{-3} M $NaNO_2$ added in eight portions at 15 min intervals, and at 37 °C, (ii) under an argon atmosphere, and (iii) under an $^{18}O_2$ atmosphere. When required, $Na^{15}NO_2$ was used in the reaction of 25 x 10^{-6} M **1a** and the mixture was worked up as above and directly analyzed by NMR and LC/MS. For kinetic experiments **1a** (2.5 x 10^{-5} M) was reacted with 1 x 10^{-3} M $NaNO_2$ added in one portion. In control experiments, the reaction was carried out under the conditions of the general procedure without added $NaNO_2$. Reaction of **1a** (3.5 x 10^{-2} M) with $NaNO_2$ (0.35 M) was also run in acetonitrile containing 2.5% acetic acid; the reaction course was followed by HPLC (eluant A). Reaction of 3,4',5-trimethoxystilbene (2.5 x 10^{-4} M) with $NaNO_2$ (1 x 10^{-3} M) was carried out at pH 3.0, and the reaction course was followed by HPLC (gradient elution: water, solvent A; acetonitrile, solvent B; from 20 to 80% B, 0-45 min; 80% B, 45-55 min). **Isolation of *rac*-(2*R*,3*R*)-3-(3,5-Dihydroxyphenyl)-2-(4-hydroxyphenyl)- 2,3-dihydrobenzofuran-5-carbaldehyde (2), (*E*)- 3,4′,5-Trihydroxy-α-nitrostilbene (3a), (*E*)-3,4 ′,5-Trihydroxy-3 ′- nitrostilbene (4),[31] (*E*)-3,4 ′,5-Trihydroxy-2,3 ′-dinitrostilbene (5), 3,5-Dihydroxybenzaldehyde, (3,5-Dihydroxyphenyl)nitromethane, 4-Hydroxybenzaldehyde, and 4-Hydroxy-3-nitrobenzaldehyde.** For preparative purposes, the reaction of **1a** with $NaNO_2$ was carried out as in the general procedure using 400 mg of starting material. After workup of the reaction mixture, the residue (380 mg) was fractionated by preparative TLC to give **3a** (R_f 0.36, 18 mg, 4% yield, >95% purity), **2** [29] (R_f 0.40, 10 mg, 2% yield, >90%purity), **4** (R_f 0.55, 5 mg, 1% yield, >98% purity), 4-hydroxybenzaldehyde (R_f 0.69, 8 mg, 4% yield), **5** (R_f 0.78, 4 mg, 1% yield, >90% purity), and 4-hydroxy-3-nitrobenzaldehyde (R_f 0.84, 4 mg, 1% yield). The fraction (5 mg) eluting at R_f 0.48 was found to consist of 3,5-dihydroxybenzaldehyde and (3,5-dihydroxyphenyl)nitromethane. **3a.** UV λ_{max}: CH_3OH, 276, 356 nm; CH_3OH/0.1 M $NaHCO_3$, pH 8, 302, 451 nm. ^1H and ^{13}C NMR: see Table 1. HR ESI-/MS: found *m/z* 272.0563 ([M - H]$^-$), calcd for $C_{14}H_{10}NO_5$ *m/z* 272.0559. **4.** UV λ_{max}: CH_3OH 303, 323, 396 nm; CH_3OH/0.1 M $NaHCO_3$, pH 8, 331, 464 nm. ^1H and ^{13}C NMR: see Table 1. ^1H NMR (CD_3OD): δ 6.20 (1H, t, *J* = 2.0 Hz), 6.49 (2H, d, *J* = 2.0 Hz), 6.96 (1H, d, *J* = 16.4 Hz), 7.01 (1H, d, *J* = 16.4 Hz), 7.13 (1H, d, *J* =8.8 Hz), 7.83 (1H, dd, *J* = 8.8, 2.0 Hz), 8.14 (d, 1H, *J* = 2.0 Hz). HR ESI-/MS: found *m/z* 272.0555 ([M - H]$^-$), calcd for $C_{14}H_{10}NO_5$ *m/z* 272.0559. **5.** UV λ_{max}: CH_3OH 300, 394 nm; CH_3OH/0.1M $NaHCO_3$, pH 8, 317, 399 nm. ^1H and ^{13}C NMR: see Table 1. HR ESI+/MS: found *m/z* 319.0561 ([M + H]$^+$), calcd for $C_{14}H_{11}N_2O_7$ *m/z* 319.0566; found *m/z* 341.0380 ([M + Na]$^+$), calcd for $C_{14}H_{10}N_2O_7Na$ *m/z* 341.0386. ***R_f* 0.48 Band.** ^1H NMR resonances for (3,5-dihydroxyphenyl)nitromethane: δ 5.48 (2H, s), 6.42 (1H, t, *J* = 2.0 Hz), 6.50 (2H, d, *J* = 2.0 Hz). ^{13}C NMR resonances for (3,5-dihydroxyphenyl)nitromethane: δ 81.8 (CH_2), 103.9 (CH), 110.6 (2 x CH), 135.0 (C), 160.8 (2 x C). LC/ESI+/MS: t_R 13.9 min, *m/z* 192 ([M + Na]$^+$). HR ESI+MS: found 192.0279 ([M + Na]$^+$), calcd for $C_7H_7NO_4Na$ *m/z* 192.0273.