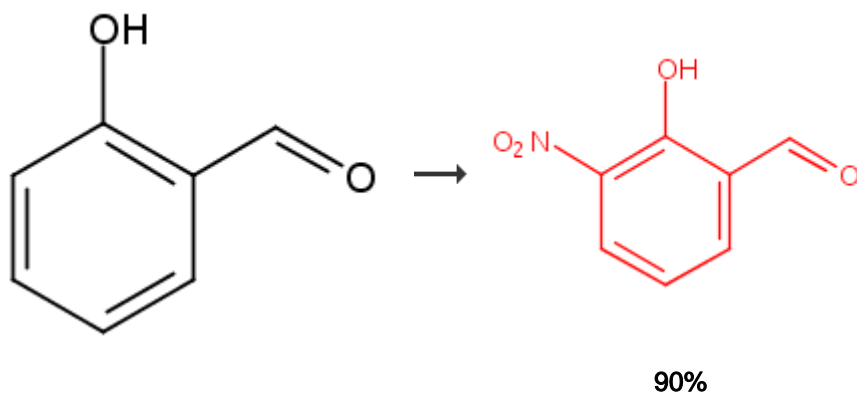
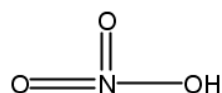


1. Single Step

[Overview](#)

Steps/Stages

1.1 R:

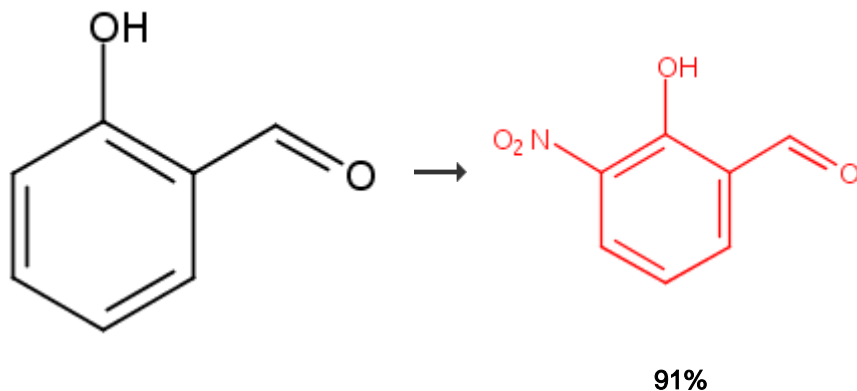
• 3 H₂O

• 1/2 Zn

C:Cyanuric trichloride, S:MeCN, 100 min, rt

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2. Single Step

[Overview](#)

Steps/Stages

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

Notes

1.1 R:AcOH, R:HNO₃

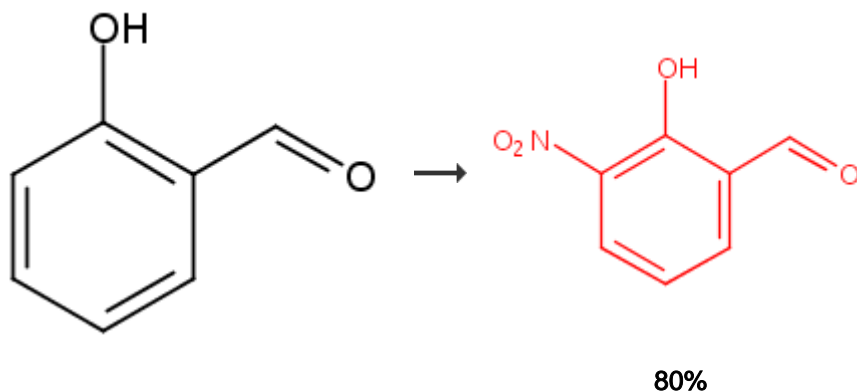
Reactants: 1, Reagents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References[Preparation of 5-nitrosalicylaldehyde ethanolamine Schiff base](#)

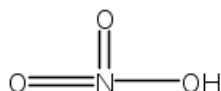
By Liu, Cuiying and Guo, Xiuying

From Huaxue Shiji, 16(6), 368, 326; 1994

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3. Single Step**Overview****Steps/Stages**

1.1 R:



• 1/2 Ni(II)

• 3 H₂O

R:Cellulose, C:Cyanuric trichloride, S:MeCN, 50 min, rt

Experimental Procedure

General/Typical Procedure: **Typical Procedure for Mononitration of Phenols** Phenol (0.094 g, 1 mmol), cellulose-supported metal nitrates (0.5 g), and TCT (0.006 g, 0.03 mmol) were stirred in 5mL of acetonitrile 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 acetonitrile (2-5 mL) and dried over anhydrous sodium sulfate, and finally the solvent was removed under vacuum (35-40°C). The crude product was treated with *n*-pentane (4-nitrophenol is insoluble in *n*-pentane), and then the *n*-pentane was evaporated by water bath (35-40°C). **2-Hydroxy-3-nitrobenzaldehyde (Entry 6, Table 3)**. Mp 107-108°C (lit.^[38] mp 105-109°C); ¹H NMR (300 MHz; CDCl₃; Me₄Si): δ 11.84 (s, br, 1H), 10.27 (s, 1H), 8.34 (d, d, *J* = 9.1, *J* = 2.9 Hz, 1H), 8.25 (d, d, *J* = 8.1, *J* = 1.7 Hz, 1H), 8.04 (d, d, *J* = 7.6, *J* = 1.7 Hz, 1H).

Notes

regioselective, green chemistry-process simplification, solid-supported reagent, cellulose-supported Ni(NO₃)₂·6H₂O prepared and used as reagent, mechanism studied, reagent recyclable, Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

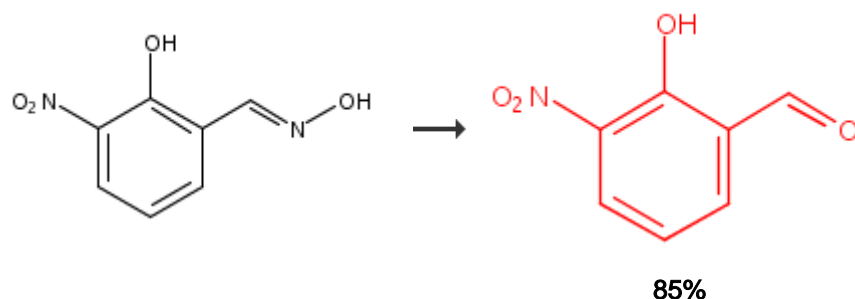
[Cellulose-supported Ni\(NO₃\)₂·6H₂O/2,4,6-trichloro-1,3,5-triazine \(TCT\) as a mild, selective, and biodegradable system for nitration of phenols](#)

By Nemati, Firouzeh et al

From Synthetic Communications, 41(20), 2985-2992; 2011

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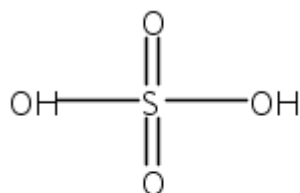
4. Single Step



Overview

Steps/Stages

1.1 R:

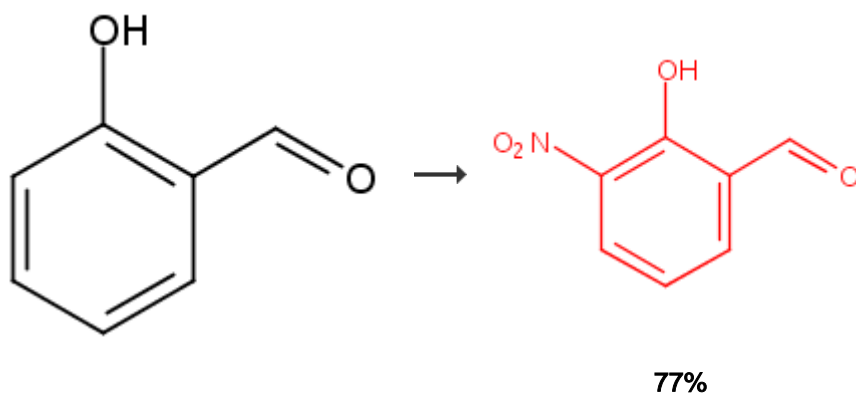


- 1/4 Zr(IV)

C:H₂O, C:SiO₂, S:Me(CH₂)₄Me, 4.5 h, reflux

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5. Single Step



Overview

Steps/Stages

Notes

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

References

[Regeneration of carbonyl compounds by cleavage of C:N bonds under mild and completely heterogeneous conditions](#)

By Shirini, F. et al

From Tetrahedron Letters, 44(40), 7463-7465; 2003

Notes

- 1.1 R:Ce(NH₄)₂(NO₃)₆, R:AcOH, C:HOCH₂CH₂OH polymer, S:H₂O, rt → 40°C; 1.6 h, 40°C
- 1.2 R:H₂O, cooled
- 1.3 R:NaOH, S:H₂O
- 1.4 R:HCl, S:H₂O, pH 4.5

regioselective, green chemistry, optimization study, optimized on amount of Ammonium cerium(IV) nitrate, catalyst, amount of catalyst, concentration of HOAc, reaction temperature, phase transfer catalyst PEG-400 used, Reactants: 1, Reagents: 5, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 4, Most stages in any one step: 4

References

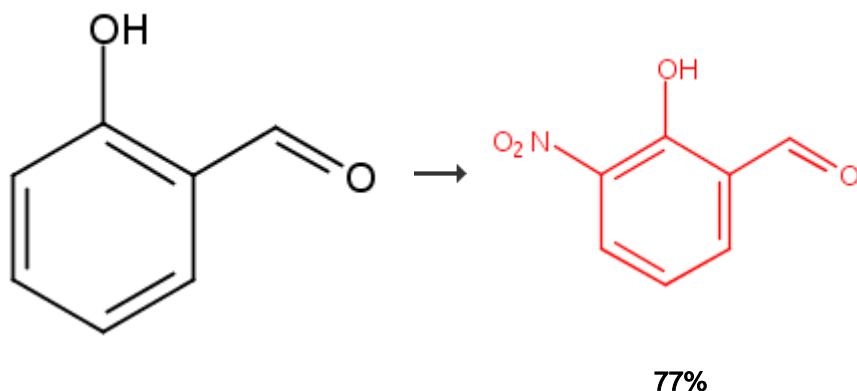
[Synthesis of 3-nitrosalicylaldehyde using polyethylene glycol as a phase transfer catalyst](#)

By Zhu, Hui-qin

From Huaxue Shijie, 50(6), 355-357; 2009

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6. Single Step



Overview

Steps/Stages

- 1.1 R:Ce(NH₄)₂(NO₃)₆, C:HOCH₂CH₂OH polymer, S:AcOH, S:H₂O, 1.2 h, 30°C

Notes

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

References

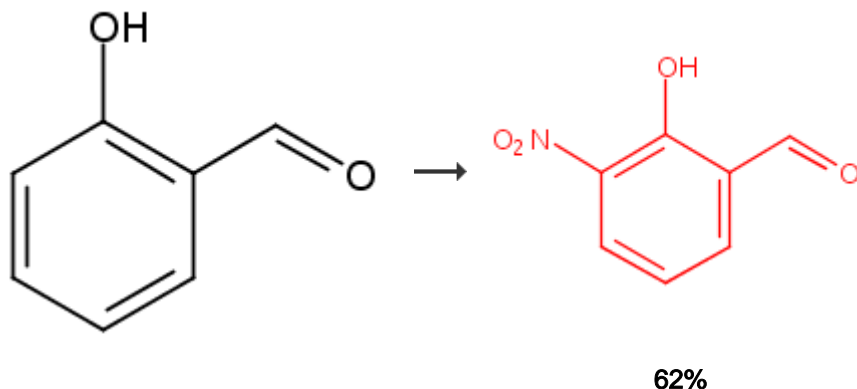
[Method for preparing 3-nitrosalicylaldehyde from salicylaldehyde and cerium ammonium nitrate](#)

By Zhu, Huiqin et al

From Faming Zhuanli Shenqing, 101020640, 22 Aug 2007

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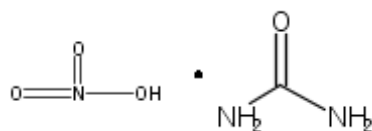
7. Single Step



Overview

Steps/Stages

1.1 R:



S:H₂O, S:MeCN, 45 min, 80°C

Notes

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

References

[Microwave-assisted synthesis of nitrophenols from the reaction of phenols with urea nitrate under acid-free conditions](#)

By Verma, Sanny et al

From Tetrahedron Letters, 55(7), 1320-1322; 2014

Reaction Protocol

Procedure

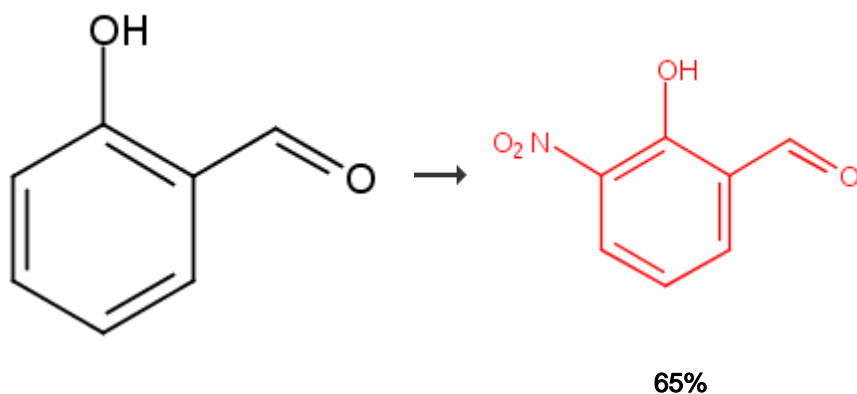
1. Mix the substituted phenol (10 mmol) and urea nitrate (10 mmol) together in acetonitrile-water (95:5, 5 ml) in a 25 ml round bottomed flask.
2. Place in a Milestone's Start SYNTH microwave reactor.

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8. Single Step



Overview

Steps/Stages

1.1 R:HNO₃, S:H₂O, -30°C; 3 min, heated

Notes

microwave irradiation, regioselective, product depends on temperature, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

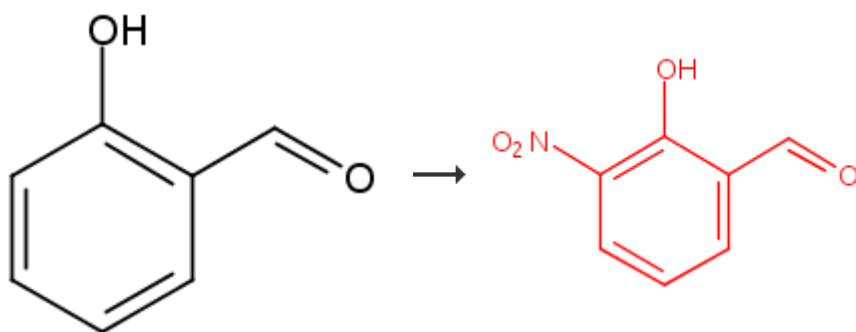
References

[Cold microwave chemistry. Synthesis using pre-cooled reagents](#)

By Bose, Ajay K. et al

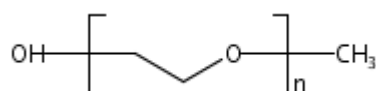
From Tetrahedron Letters, 47(19), 3213-3215; 2006

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9. Single Step**Overview****Steps/Stages**

1.1 R:Ce(NH₄)₂(NO₃)₆

R:



S:AcOH

Notes

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

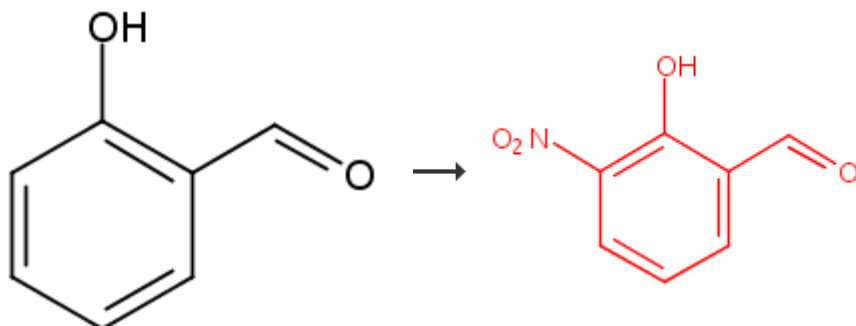
References

[Study on synthesis of 3-nitrosalicylaldehyde Schiff bases and their antibacterial activity](#)

By Zhu, Hui-qin et al

From Huaxue Shijie, 52(12), 737-739; 2011

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10. Single Step

[Overview](#)**Steps/Stages**

1.1 R:HNO₃, S:AcOH, < 15°C

Notes

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

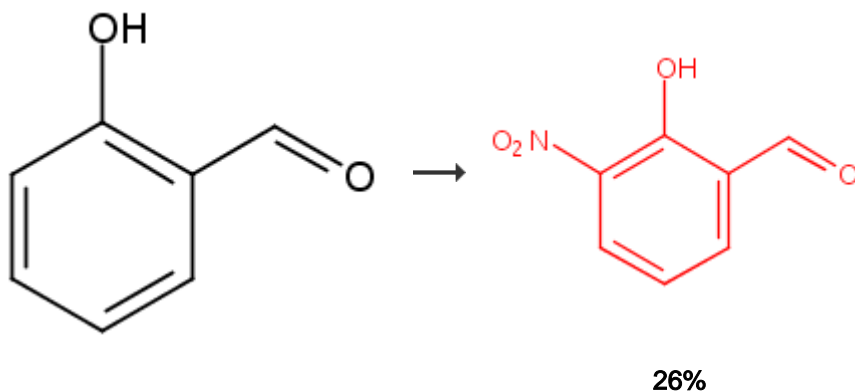
References

[Synthesis of new organochromium compounds](#)

By Zhang, Hua et al

From Shanghai Gongcheng Jishu Daxue Xuebao, 19(4), 309-313; 2005

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11. Single Step[Overview](#)**Steps/Stages**

1.1 R:AcOH, R:HNO₃, S:H₂O, 0°C; 2 h, 0°C → rt; 5 h, 40°C

Notes

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

References

[Preparation of 2,4-diamino-6,7-dihydro-5H-pyrrolo\[2,3\]pyrimidine derivatives as FAK and/or Pyk2 inhibitors](#)

By Xiao, Dengming et al

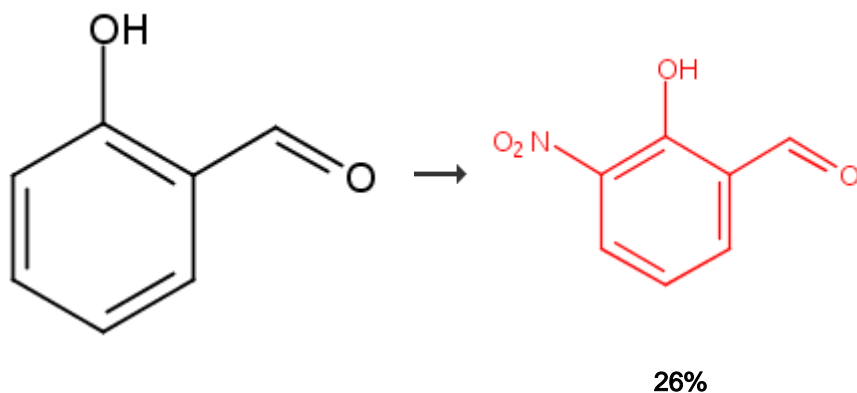
From PCT Int. Appl., 2012092880, 12 Jul 2012

Experimental Procedure

Step A: 2-hydroxy-3-nitrobenzaldehyde To a solution of 2-hydroxybenzaldehyde (5.0 g, 41 mmol) in acetic acid (50 mL) at 0 °C was added nitric acid (65 %, 4 g) dropwise. The reaction mixture was slowly warmed to room temperature for 2 hours and then heated at 40 °C for another 5 hours. The resulting mixture was poured into ice (75 g) and water (500 g). The precipitates were filtrated and purified by silica gel chromatography to afford the product 2-hydroxy-3-nitrobenzaldehyde. Yield 1.8 g, 26 %. ¹H NMR (400 MHz, CDCl₃) δ ppm 11.44 (s, 1H), 10.42 (s, 1H), 8.34-8.37 (dd, 1H, *J* = 2.0 Hz, 8.4 Hz), 8.10-8.13 (dd, 1H, *J* = 2.0 Hz, 7.6 Hz), 7.12-7.16 (t, 1H, *J* = 8.0 Hz).

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12. Single Step

[Overview](#)

Steps/Stages

- 1.1 R:AcOH, R:HNO₃, S:H₂O, 0°C; 0°C → rt; 2 h, rt; rt → 40°C; 5 h, 40°C
- 1.2 S:H₂O, cooled

Notes

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

References

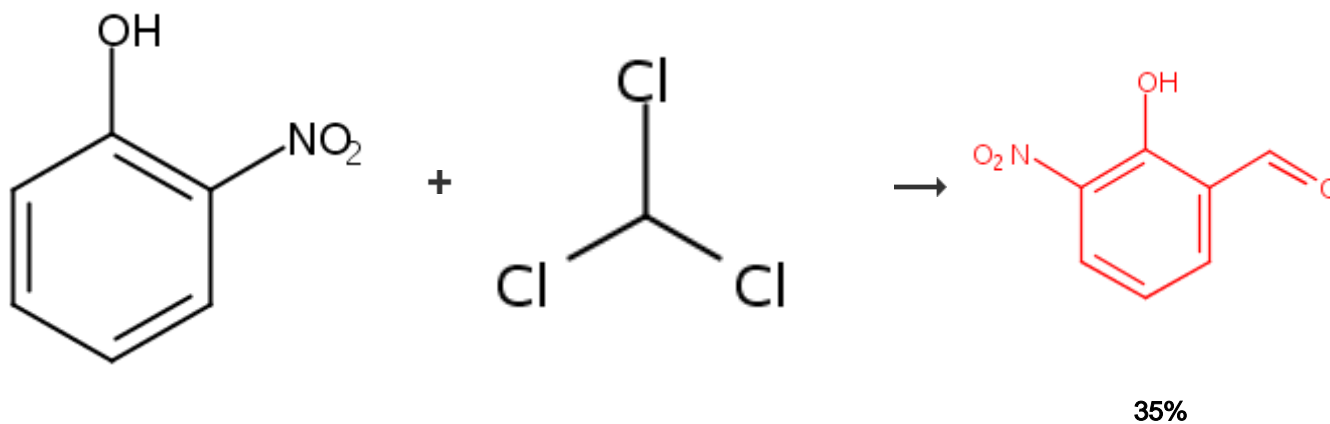
[Preparation of 2,4-diamino-6,7-dihydro-5H-pyrrolo\[2,3\]pyrimidine derivatives as FAK/PTK2B inhibitors](#)

By Xiao, Dengming et al

From Faming Zhuanli Shenqing, 102093364, 15 Jun 2011

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13. Single Step

[Overview](#)

Steps/Stages

Notes

1.1 R:NaOH, S:H₂O

1.2

Reimer-Tieman method, Reactants: 2,
Reagents: 1, Solvents: 1, Steps: 1, Stages: 2,
Most stages in any one step: 2

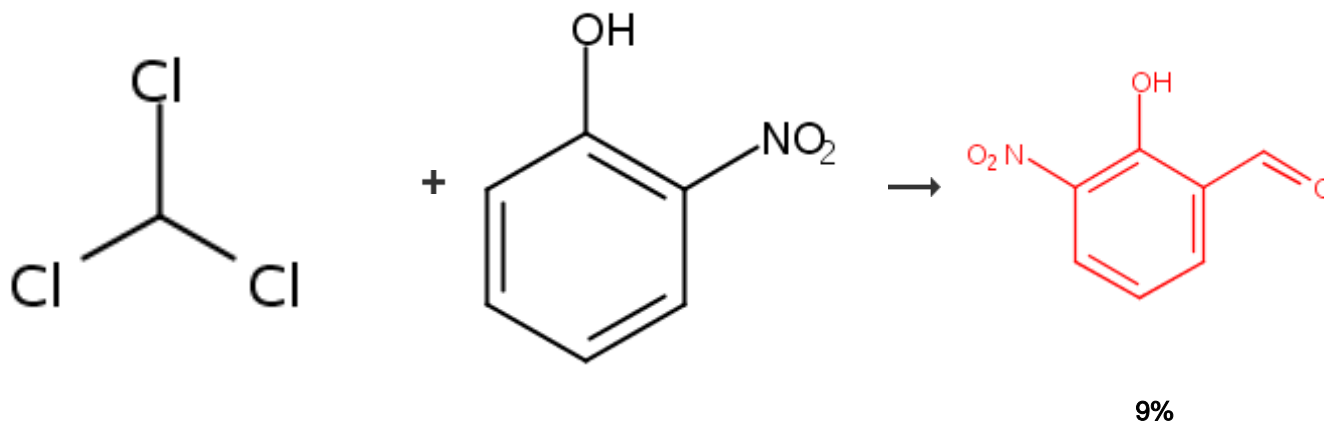
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[Thermochromic and photochromic properties of some new spirocyan systems](#)

By Feng, K-C. and Griffiths, J.

From *Advances in Colour Science and Technology*, 4(1), 12-20; 2001

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14. Single Step[Overview](#)**Steps/Stages**1.1 S:CHCl₃, S:H₂O**Notes**

regioselective, Alkali, Aq. Hydroxide, CHCl₃, Alkylation, C-Alkylation, C-Formylation, Carbene intermediate, Cleavage, Hydrolysis, Selective, Reactants: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

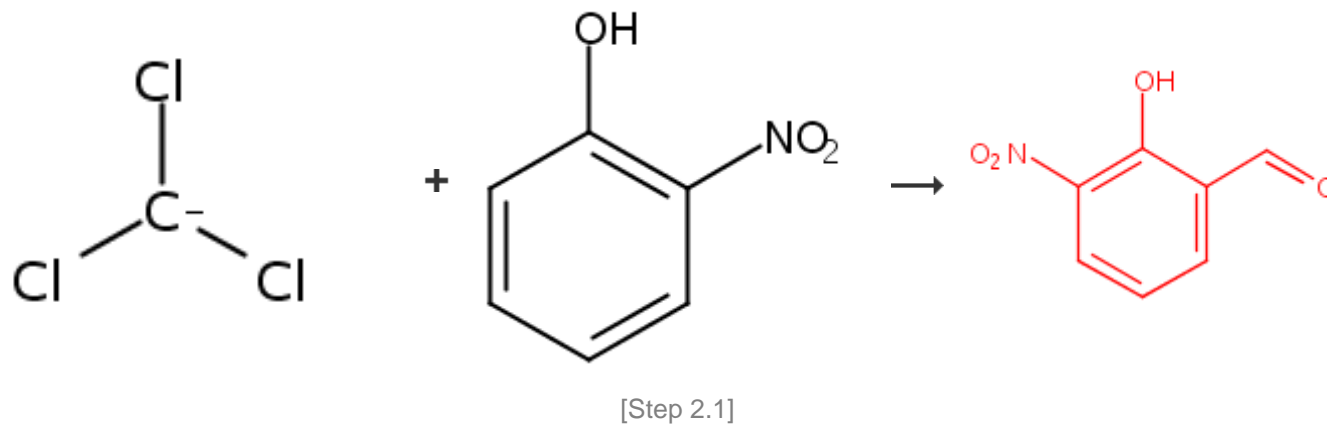
[The Reimer-Tiemann reaction](#)

By Wynberg, Hans and Meijer, Egbert W.

From *Organic Reactions* (Hoboken, NJ, United States), 28, No pp. given; 1982

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15. 2 Steps



Overview

Steps/Stages

- 1.1 R:H₂O
2.1 S:CHCl₃, S:H₂O

Notes

1) H₂O, 2) regioselective, Alkali, Aq. Hydroxide, CHCl₃, Alkylation, C-Alkylation, C-Formylation, Carbene intermediate, Cleavage, Hydrolysis, Selective, Reactants: 2, Reagents: 1, Solvents: 2, Steps: 2, Stages: 2, Most stages in any one step: 1

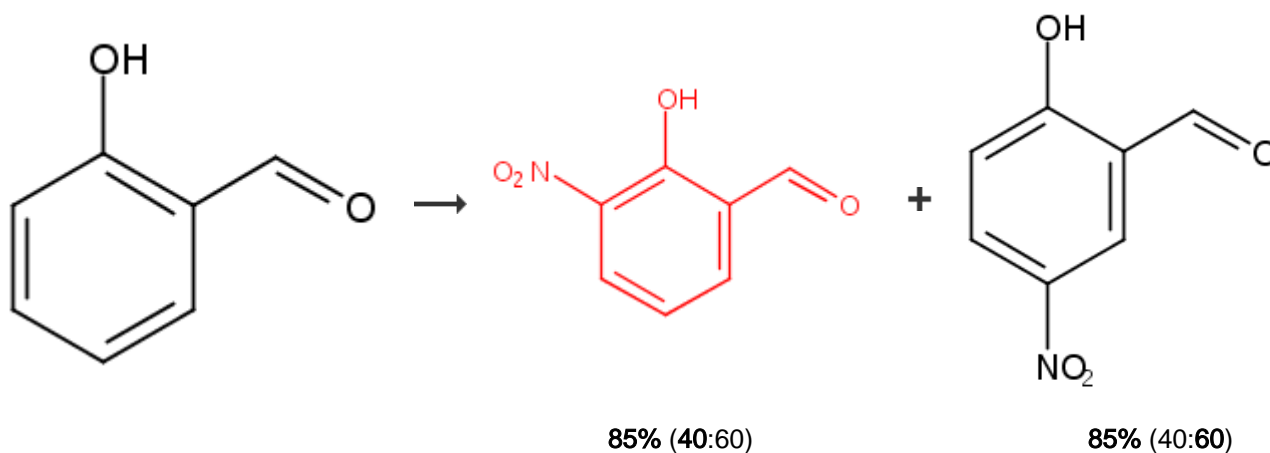
References

[The Reimer-Tiemann reaction](#)

By Wynberg, Hans and Meijer, Egbert W. From Organic Reactions (Hoboken, NJ, United States), 28, No pp. given; 1982

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16. Single Step



Overview

Steps/Stages

Notes

- 1.1 R:NH₄NO₃ (clay-supported), rt → 0°C
 1.2 R:HClO₄, 120 min, 35°C
 1.3 R:NaHCO₃, S:H₂O, neutralized

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

References

[Clay supported ammonium nitrate "Clayan". A new reagent for selective nitration of arenes](#)

By Meshram, H. M. et al

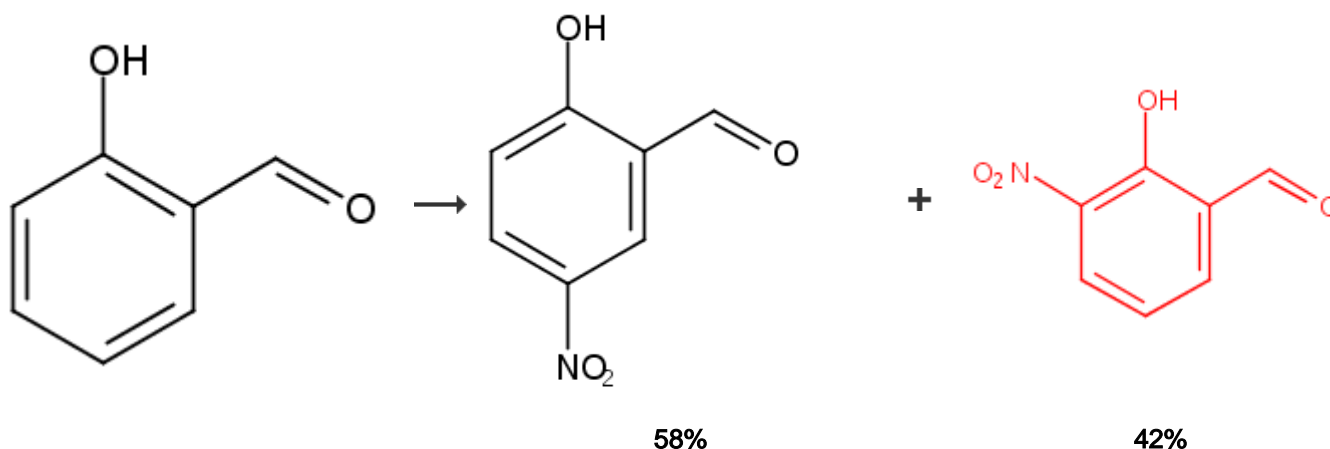
From Synthetic Communications, 33(14), 2497-2503; 2003

Experimental Procedure

General/Typical Procedure: **Typical Experimental Procedure** Arene (1 mmol) was mixed with "Clayan"^[3] (192 mg, 1.2 mmol of ammonium nitrate present in the reagent), cooled to 0°C, and perchloric acid (3 mL, 60% w/v) was added dropwise. Slurry was stirred for the stipulated time (see table) and the reaction was monitored by tlc. After completion of the reaction, reaction mixture was diluted with water, neutralized with bicarbonate solution (10%), filtered and leached with ethylacetate (2 x 10 mL). Organic layer was separated and dried over magnesium sulphate. Evaporation of the solvent gave the crude product, which was column purified by ethyl acetate:hexane mixture (20:80). Entry no. 13, yield 85%.

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17. Single Step



Overview

Steps/Stages

- 1.1 S:22113-86-6, > 1 min, rt
 1.2 R:O(SO₂CF₃)₂, 0°C; 30 min, 0°C → rt

Notes

chemoselective, ionic liquid used, regioselective, safety (vigorous reaction), Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

[Ethylammonium Nitrate \(EAN\)/Tf₂O and EAN/TFAA: Ionic Liquid Based Systems for Aromatic Nitration](#)

By Aridoss, Gopalakrishnan and Laali, Kenneth K.

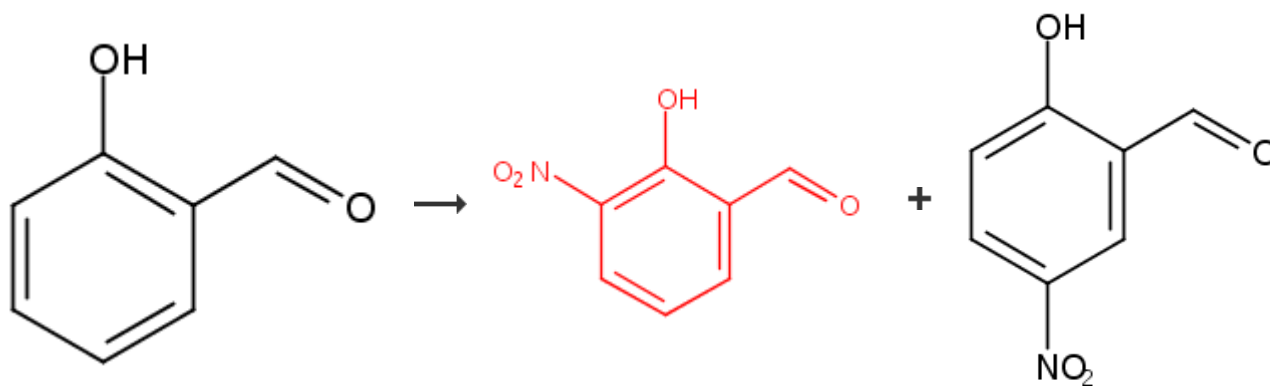
From Journal of Organic Chemistry, 76(19), 8088-8094; 2011

Experimental Procedure

General/Typical Procedure: **General Procedure.** The desired aromatic compound (1 mmol) was added to EAN (typically 5 mmol for nitration of liquid substrates and ~10 mmol for nitration of solids) under nitrogen at room temperature and stirred for a few minutes. Tf₂O (triflic anhydride) or TFAA (trifluoroacetic anhydride) (1 mmol) was added slowly with stirring while the reaction mixture was kept at low temperature (as mentioned in Tables 1 and 3-5). The progress of the reaction was monitored by GC and/or GC-MS. The reaction mixture was extracted three to four times with dry ether, chloroform-hexane mixture (1:2), or ethyl acetate-hexane mixture (2:6). The combined extracts were washed with bicarbonate solution (8%) and brine and dried over MgSO₄. Removal of solvents under reduced pressure gave the crude product. Isomer distributions were determined by GC, GC MS and/or by ¹H NMR. In selected cases, the major product(s) were isolated and purified by column chromatography (4:1 ethyl acetate/hexane). To obtain optimal conversions in nitration of deactivated arenes, it is imperative that EAN, Tf₂O and TFAA are dry and fresh (substantially lower yields or no reaction were observed with older reagents in bottles/flasks that had been repeatedly opened!) **2-Hydroxy-nitrobenzaldehydes (26):** NMR chemical shift values of the respective isomers were determined directly from the isomeric mixture. **3-Nitro** compound: yield 58%; **5-Nitro** compound : yield 48%. **3-Nitro:** ¹H NMR (500 MHz, CDCl₃, 25 °C): δ 7.14 (t, *J* = 7.95 Hz, 1H), 8.11 (dd, *J* = 1.7 Hz, *J* = 7.6 Hz, 1H), 8.41 (dd, *J* = 2.9 Hz, *J* = 9.2 Hz, 1H), 10.41 (s, 1H), 11.44 (s, 1H); ¹³C NMR (125 MHz, CDCl₃, 25 °C): δ 119.5, 125.6, 131.5, 135.5, 137.3, 156.7, 189.5; GC/MS (EI) *m/z* 167 (M⁺, 100%), 149, 137, 120, 109, 92, 81, 65, 46. **5-Nitro:** ¹H NMR (500 MHz, CDCl₃, 25 °C): δ 7.13 (d, *J* = 9.3 Hz, 1H), 8.35 (dd, *J* = 1.7 Hz, *J* = 8.3 Hz, 1H), 8.57 (d, *J* = 2.7 Hz, 1H), 10.00 (s, 1H), 11.60 (s, 1H); ¹³C NMR (125 MHz, CDCl₃, 25 °C): δ 119.2, 119.9, 129.9, 131.8, 140.8, 166.3, 195.6; GC/MS (EI) *m/z* 167 (M⁺), 149 (100%), 120, 91, 77, 63, 39.

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18. Single Step



Overview

Steps/Stages

1.1 R:HNO₃, S:H₂O, S:AcOH, 0.5 h, 0-5°C

Notes

exothermic, combined yield = 90%, 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

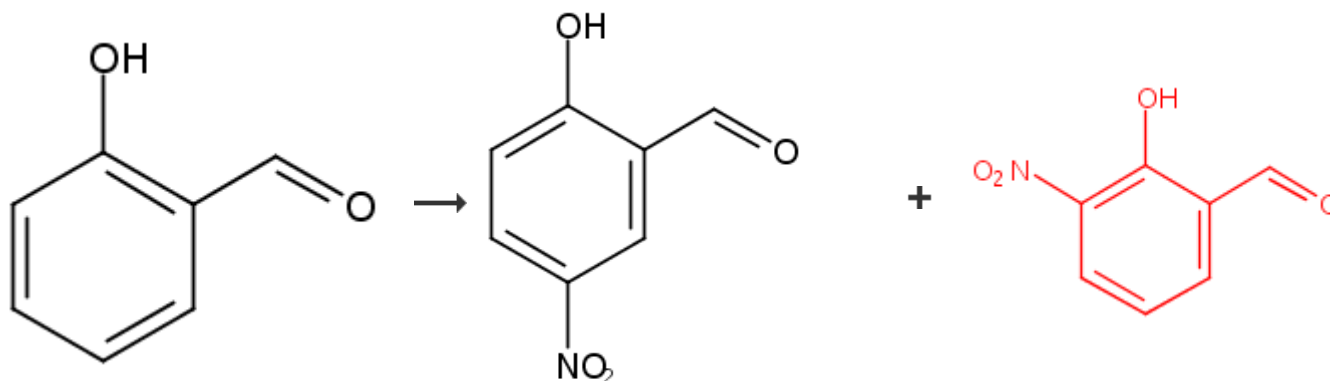
From Journal of Thermal Analysis and Calorimetry, 112(3), 1587-1599; 2013

Experimental Procedure

Nitration of 2-hydroxy benzaldehyde. Reaction was performed in two steps according to the literature. 10 mL 2-hydroxy benzaldehyde and 10 mL HNO₃ (63 %) were dissolved in 50 mL of CH₃COOH and the mixture was stirred for half an hour in ice-water bath at 0-5 °C. After that, the reaction vessel was kept at room temperature and the solution became warmer because of the exothermic nitration reaction. Before starting to boil, this solution was poured into a 250 mL of ice-water mixture. Mixture of 3-nitro-2-hydroxy benzaldehyde and 5-nitro-2-hydroxy benzaldehyde were the precipitates which were then filtered and air dried. 3-nitro-2-hydroxy benzaldehyde. 5-nitro-2-hydroxy benzaldehyde. Yield of this reaction is found to be 90 %. 3-nitro-2-hydroxy benzaldehyde: Melting point 109 °C, Important IR Data cm⁻¹ ν_{O-H} = 2804 ν_{C=O} = 1653 ν_{C=C} = 1631 ν_{N=O} = 1334 ν_{C-H(Ar)} = 3091-3068 ν_{C-H(Alid)} = 2887 δ_{C-H(Ar)} = 751, elemental analysis Expected C% = 50:31; H = 3:01; N = 8:37 Found C% = 49:80; H = 3:36; N = 8:12. 5-nitro-2-hydroxy benzaldehyde: Melting point 127 °C, Important IR Data cm⁻¹ ν_{O-H} = 2812 ν_{C=O} = 1654 ν_{C=C} = 1625 ν_{N=O} = 1331 ν_{C-H(Ar)} = 3068-3047 ν_{C-H(Alid)} = 2887 δ_{C-H(Ar)} = 748, elemental analysis Expected C% = 50:31; H = 3:01; N = 8:37 Found C% = 50:17; H = 3:41; N = 7:86.

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19. Single Step



Overview

Steps/Stages

- 1.1 R:AcOH, R:HNO₃, S:H₂O, 1-5°C; 5°C → 40°C
- 1.2 R:NaOH, S:H₂O, 6 h, pH 8-9
- 1.3 R:HCl, S:H₂O, pH 4-5

Notes

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

References

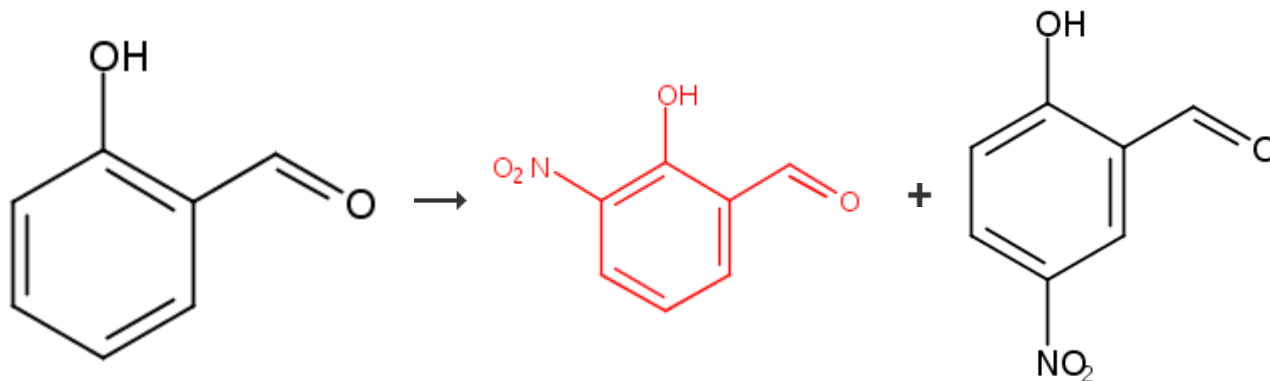
[Synthesis and characterization of Schiff base complexes functionalized MCM-41 mesoporous molecular sieves](#)

By Huo, Yong-qian et al

From Xibei Daxue Xuebao, Ziran Kexueban, 39(6), 992-997; 2009

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20. Single Step



[Overview](#)

Steps/Stages

1.1 R:HNO₃ •NO₂, S:AcOH, < 15°C

Notes

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

References

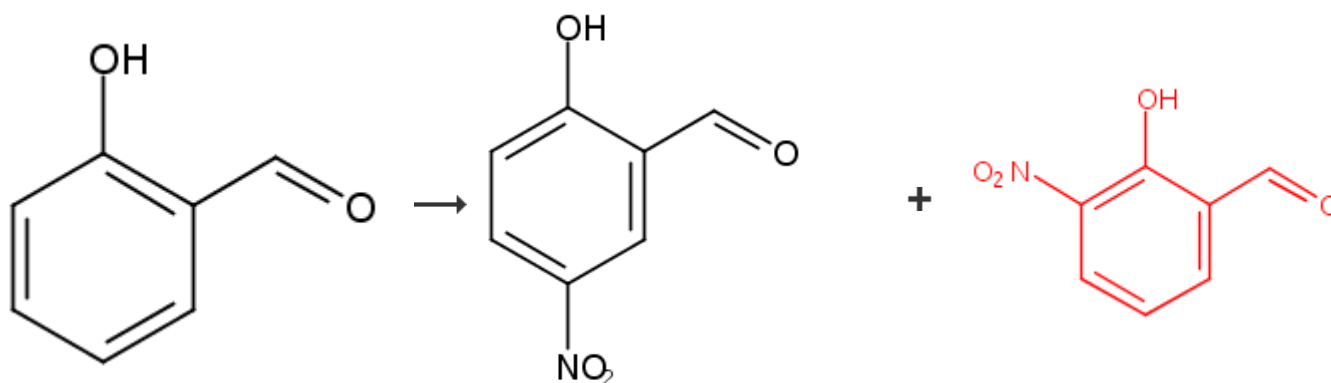
[Synthesis and characterization of four chromium\(III\) mixed-ligand complexes with amino acid schiff base](#)

By Zhang, Hua et al

From Huaxue Shiji, 31(4), 283-284, 302; 2009

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21. Single Step



[Overview](#)

Steps/Stages

Notes

1.1 R:HNO₃•NO₂, S:AcOH, 2.5-3 h, 10°C; 10°C → 45°C; 4 h, 45°C

regioselective, fuming nitric acid used, overall yield 89%, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

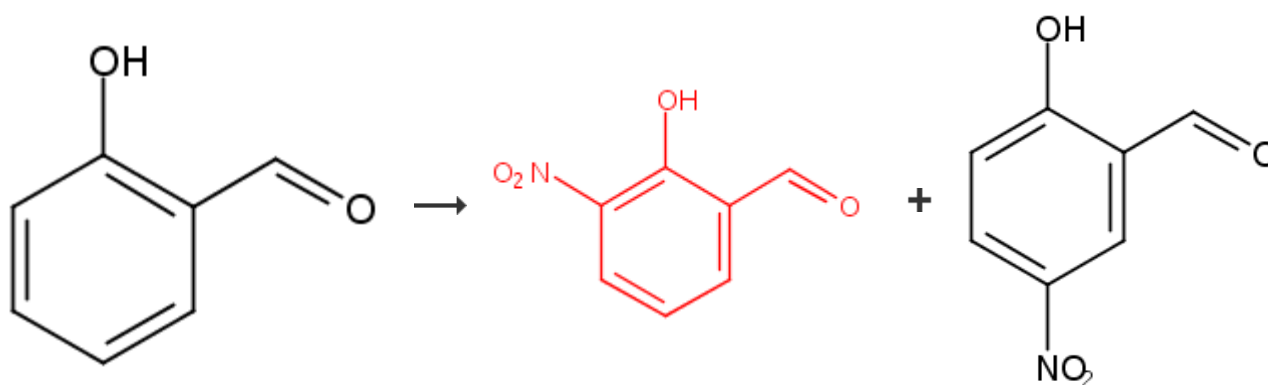
[Synthesis and spectral properties of bis\(substituted salicylaldehyde\)ethylenediamine Schiff-bases](#)

By Zhang, Ying-ju et al

From Ranliao Yu Ranse, 42(5), 38-40, 18; 2005

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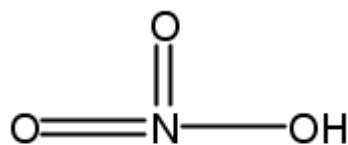
22. Single Step



Overview

Steps/Stages

1.1 R:



• 1/3 Al

S:EtOH, 8 h, reflux

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23. Single Step

Notes

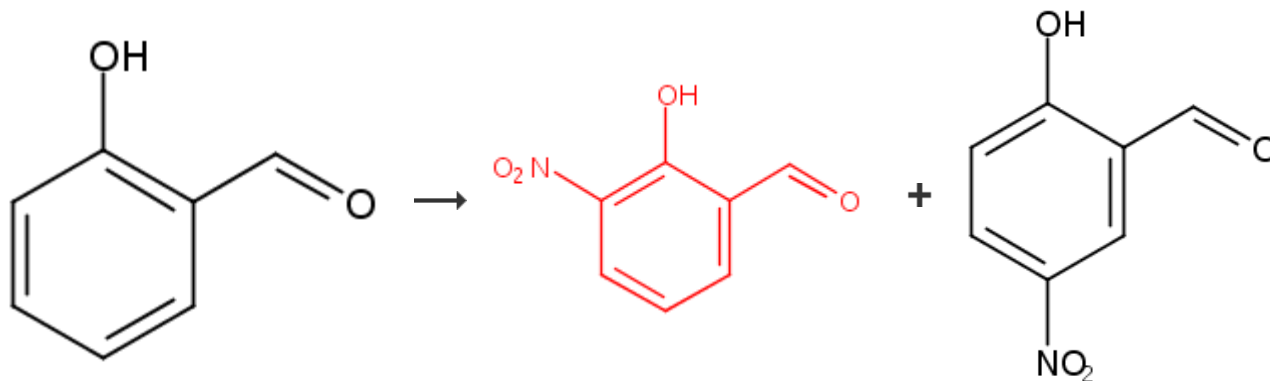
regioselective, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

[Process for nitration of phenols with aluminum nitrate](#)

By Gou, Shaohua and Hu, Dahua

From Faming Zhuanli Shenqing, 1736976, 22 Feb 2006



[Overview](#)

Steps/Stages

1.1

Notes

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

References

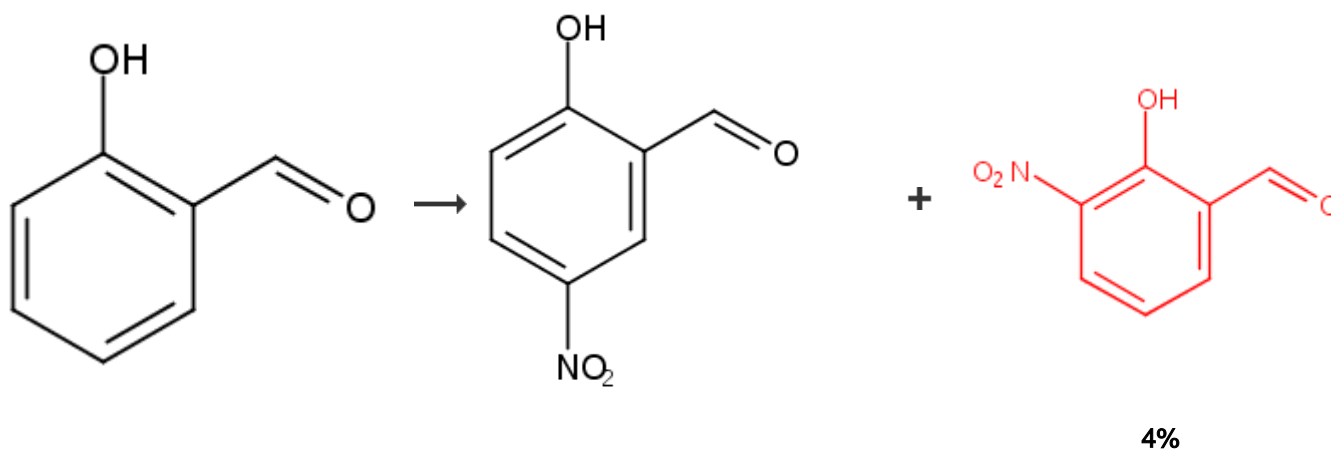
[\(-\)-\(R,R\)-N,N'-bis\(3-nitrosalicylidene\)-1,2-cyclohexanediamine as a new host compound for aromatic guests through CH/ \$\pi\$ interactions](#)

By Rafii, Esfandiar et al

From ARKIVOC (Gainesville, FL, United States), (10), 86-94; 2005

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24. Single Step



[Overview](#)

Steps/Stages

Notes

1.1

no experimental detail, literature preparation,
Reactants: 1, Steps: 1, Stages: 1, Most stages
in any one step: 1

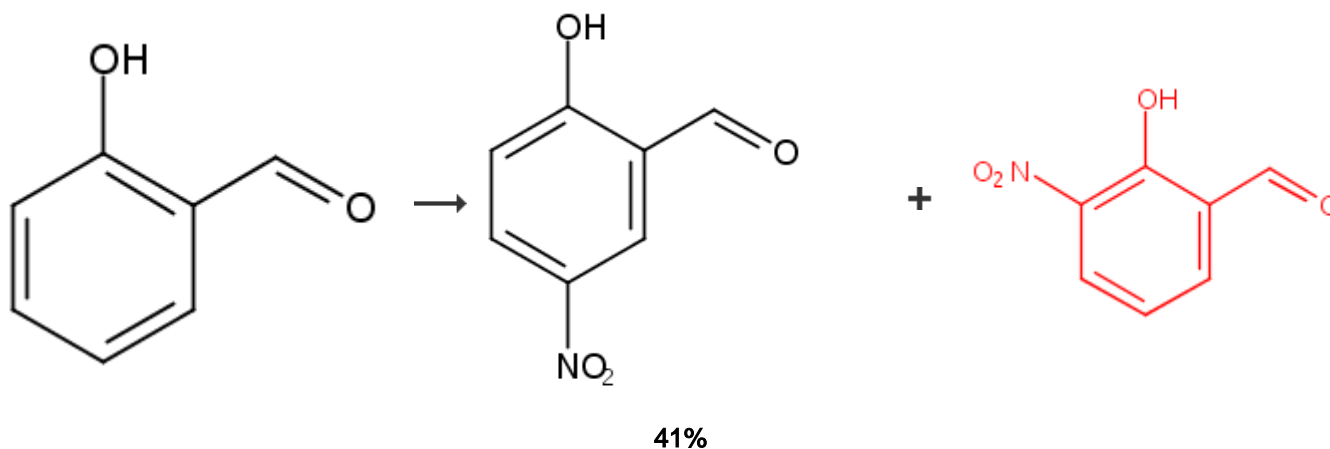
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[Decoloration rates of a photomerocyanine dye as a visual probe into hydrogen bonding interactions](#)

By Ciampi, Simone et al

From Chemical Communications (Cambridge, United Kingdom), 51(23), 4815-4818; 2015

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25. Single Step[Overview](#)**Steps/Stages**

- 1.1 R:AcOH, R:HNO₃, S:H₂O, 5°C; 2 h, 20°C; 20°C → 30°C; 30°C → 45°C; 1.5 h, 45°C
- 1.2 R:H₂O, overnight, cooled
- 1.3 R:NaOH, S:H₂O, overnight, 40°C
- 1.4 R:HCl, S:H₂O, pH 3

Notes

regioselective, Reactants: 1, Reagents: 5, Solvents: 1, Steps: 1, Stages: 4, Most stages in any one step: 4

References

[Synthesis of 3,3-dimethyl-N-\(2-methylacryloyloxyethyl\)-6'-nitrospiroindolinebenzopyran](#)

By He, Wei et al

From Huaxue Shiji, 26(6), 327-328, 368; 2004

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