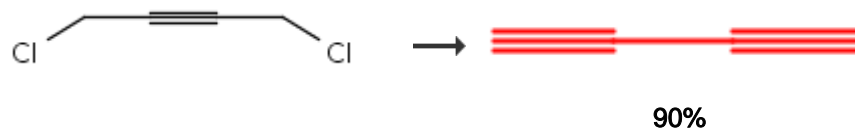


**1. Single Step**[Overview](#)**Steps/Stages**

1.1 R:KOH, S:H<sub>2</sub>O, S:DMSO

**Notes**

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

**References**

[A detailed procedure for the preparation of butadiyne](#)

By Verkruijsse, H. D. and Brandsma, L.

From *Synthetic Communications*, 21(5), 657-9; 1991

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

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

1.1 R:KOH, S:DMSO, 30 min, 70°C

1.2 30 min, 70°C

1.3 S:THF, -78°C

**Notes**

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

**References**

[Synthesis of Neutral Molecular Squares Composed of Bis\(phosphine\)platinum Corner Units and Dialkynyl Linkers. Solid-State Characterization of \[Pt\(μ-C≡CC≡C\)\(dppp\)\]<sub>4</sub>](#)

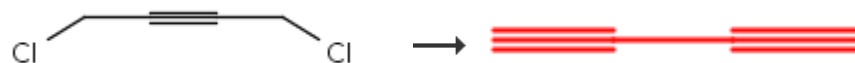
By Janka, Mesfin et al

From *Organometallics*, 23(19), 4382-4390; 2004

**Experimental Procedure**

**Preparation of Butadiyne.**<sup>44</sup> KOH (9.0 g, 0.08 mol), water (20.0 mL), and DMSO (5.0 mL) were heated to 70 °C for 30 min in a three-necked flask equipped with a condenser and a dropping funnel. The top of the condenser was connected, via a tube filled with CaCl<sub>2</sub>, to a trap containing dry THF, which was cooled to -78 °C. 1,4-Dichloro-2-butyne (4.0 mL, 0.04 mol) was added dropwise over a period of 30 min, while the temperature was maintained at 70 °C. A stream of argon was passed through the apparatus, which forced the butadiyne into the cold THF trap. The THF solution was stored at -45 °C in a sealed container. The weight increase of the trap corresponded to an 80% yield. The material could be stored for at least 3 days without significant deterioration. **Butadiyne**, yield 80%.

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**3. Single Step**

[Overview](#)**Steps/Stages**1.1 S:EtOH, S:C<sub>5</sub>H<sub>5</sub>N**Notes**

Classification: Elimination;  
Dehydrochlorination; Isomerisation; #  
Conditions: NaOH; pyridine EtOH, Reactants:  
1, Solvents: 2, Steps: 1, Stages: 1, Most  
stages in any one step: 1

**References**

[The chemistry of the acetylenes. I. Syntheses starting with diacetylene](#)

By Herbertz, Theo

From *Chemische Berichte*, 85, 475-82; 1952

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**4. Single Step**[Overview](#)**Steps/Stages**1.1 R:O<sub>2</sub>, C:Au, S:m-Dichlorobenzene, rt, 5 bar; 18 h, 170°C**Notes**

solid-supported catalyst, catalyst on carbon,  
Reactants: 1, Reagents: 1, Catalysts: 1,  
Solvents: 1, Steps: 1, Stages: 1, Most stages  
in any one step: 1

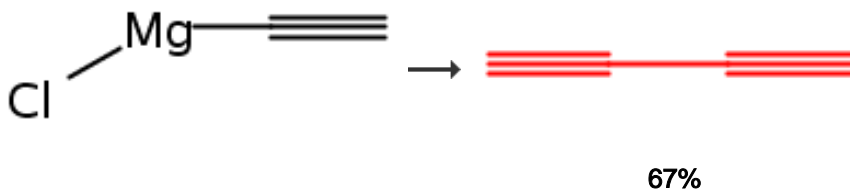
**References**

[Partially oxidized gold nanoparticles: A catalytic base-free system for the aerobic homocoupling of alkynes](#)

By Boronat, Mercedes et al

From *Journal of Catalysis*, 315, 6-14; 2014

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

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

1.1 R:ClCH<sub>2</sub>CH<sub>2</sub>Cl, C:MnCl<sub>2</sub>, S:THF, 25°C; 12 h, 25°C

1.2 R:MeOH, 25°C

dropwise addition of Grignard reagent,  
Reactants: 1, Reagents: 2, Catalysts: 1,  
Solvents: 1, Steps: 1, Stages: 2, Most stages  
in any one step: 2

### References

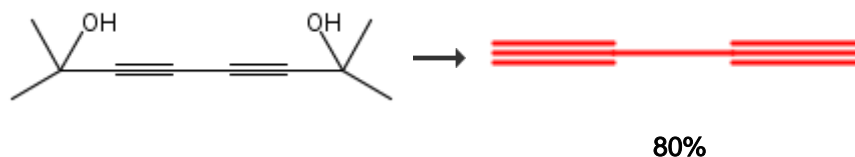
[Manganese-catalyzed oxidative homo-coupling of aryl Grignard chlorides](#)

By Zhou, Zhiming and Xue, Weizhe

From Journal of Organometallic Chemistry, 694(5), 599-603; 2009

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 6. Single Step



#### Overview

### Steps/Stages

1.1 S:Xylene

### Notes

Classification: Hydrolysis; C-Dealkylation; #  
Conditions: NaOH xylene, Reactants: 1,  
Solvents: 1, Steps: 1, Stages: 1, Most stages  
in any one step: 1

### References

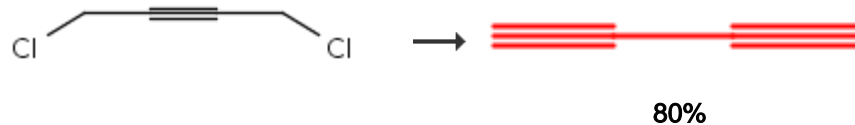
[Improved laboratory method for preparation of diacetylene](#)

By Tedeschi, R. J. and Brown, A. E.

From Journal of Organic Chemistry, 29(7), 2051-3; 1964

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 7. Single Step



#### Overview

### Steps/Stages

### Notes

1.1 S:MeOH

Classification: Elimination;  
 Dehydrochlorination; Isomerisation; #  
 Conditions: NaOH; MeOH; boil 10mn,  
 Reactants: 1, Solvents: 1, Steps: 1, Stages: 1,  
 Most stages in any one step: 1

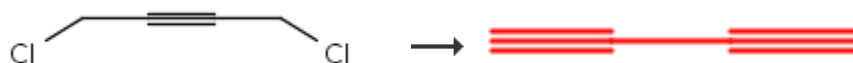
**References**

[Reduction of sulfur-containing heterocyclic compounds with lithium aluminum hydride](#)

By Angelini, Carlo et al

From *Annali di Chimica (Rome, Italy)*, 46, 235-42; 1956

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

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

1.1 R:KOH, S:H<sub>2</sub>O, S:DMSO, rt → 75°C

**Notes**

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

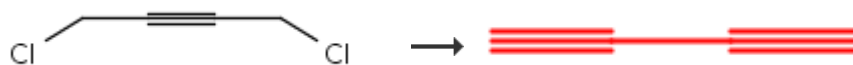
**References**

[Methods of preparing dicarbonyl compounds from biomass waste](#)

By Klein, Josef Peter

From *PCT Int. Appl.*, 2015060862, 30 Apr 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

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

1.1 R:KOH, S:H<sub>2</sub>O, S:Dioxane, 80-100°C

**Notes**

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

**References**

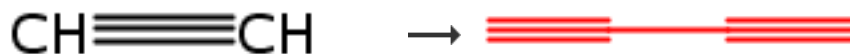
[Photodissociation Dynamics of Diacetylene Rydberg States](#)

By Wang, Hongzhen et al

From *Journal of Physical Chemistry A*, 119(46), 11313-11319; 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 10. Single Step



#### Overview

#### Steps/Stages

1.1

#### Notes

no experimental detail, gas phase, Ne-He carrier gas used, Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

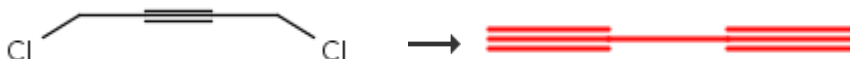
#### References

[Spectroscopy and Dynamics of Jet-Cooled Polyynes in a Slit Supersonic Discharge: Sub-Doppler Infrared Studies of Diacetylene HCCCCH](#)

By Chang, Chih-Hsuan and Nesbitt, David J.  
From Journal of Physical Chemistry A, 119(28), 7940-7950; 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 11. Single Step



#### Overview

#### Steps/Stages

1.1 R:KOH, S:H<sub>2</sub>O, S:DMSO, 50°C

#### Notes

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

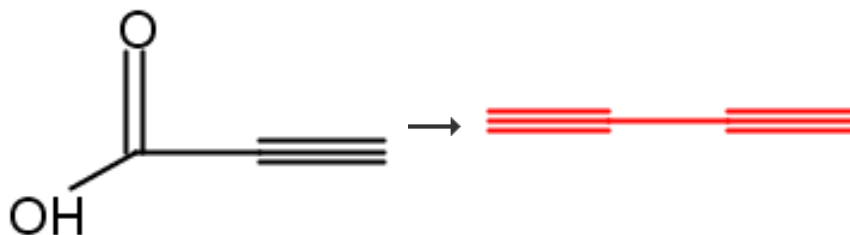
#### References

[Kinetics of the Reactions of Hydroxyl Radicals with Diacetylene and Vinylacetylene](#)

By Sommerer, Joerg and Olzmann, Matthias  
From Zeitschrift fuer Physikalische Chemie (Muenchen, Germany), 229(4), 495-505; 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 12. Single Step



### Overview

#### Steps/Stages

1.1 R:CoCl<sub>2</sub>, S:MeOH, rt

#### Notes

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

#### References

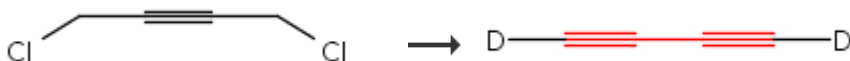
[Cobalt-Mediated Decarboxylative Homocoupling of Alkynyl Carboxylic Acids](#)

By Leeming, Michael G. et al

From Australian Journal of Chemistry, 67(5), 701-710; 2014

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

#### 13. Single Step



### Overview

#### Steps/Stages

1.1 R:KOD, S:O=S(CD<sub>3</sub>)<sub>2</sub>, S:D<sub>2</sub>O, 15 min, 75°C

#### Notes

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

#### References

[Accessing Long-Lived Disconnected Spin-1/2 Eigenstates through Spins > 1/2](#)

By Claytor, Kevin et al

From Journal of the American Chemical Society, 136(43), 15118-15121; 2014

### Experimental Procedure

*Diacetylene-d2* 1,4-dichloro-2-butyne (10g, 82 mmol) was added drop wise over 15 minutes to a stirred, heated (75°C, oil bath temperature) mixture of DMSO-d<sub>6</sub> (8 mL) and 40% KOD in D<sub>2</sub>O (30 mL). The head space was swept with a gentle stream of argon. The argon/product gas mixture was passed through an empty (to allow visual confirmation of product formation) dry ice/acetone cooled trap (10 mL Schlenk flask). Colorless crystals of the product formed within 2-3 minutes in the receiving flask. Following complete addition of 1,4-dichloro-2-butyne to the reaction mixture, argon was swept through the system for an additional 20 minutes. After which time the neck and side arm port of the Schlenk flask were septum sealed under argon and freshly distilled (P<sub>2</sub>O<sub>5</sub>) CDCl<sub>3</sub> (1 mL) was added. The flask was transferred to an ice water bath. Within a few minutes in the bath, and with some swirling, a clear, colorless solution was obtained. An aliquot (~700 uL) was removed and transferred to a septum sealed NMR tube under argon. The remainder of the reaction mixture stored at -80°C under an atmosphere of argon.

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

#### 14. Single Step



#### Overview

##### Steps/Stages

- 1.1 S:H<sub>2</sub>O, 4 min, 70°C; 70°C → rt  
1.3

##### Notes

photochemical, ultrasound (substage 1), ultraviolet irradiation, 254nm (substage 3), irradiation time is several seconds (substage 3), mixed with silicon polymer in stage 2, Reactants: 1, Solvents: 1, Steps: 1, Stages: 3, Most stages in any one step: 3

##### References

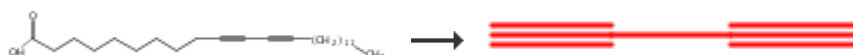
[Biosensor compositions including a polydiacetylene material and their use in detecting microbes or microbial products](#)

By Awdeh, Richard

From PCT Int. Appl., 2014052794, 03 Apr 2014

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

#### 15. Single Step



#### Overview

##### Steps/Stages

- 1.1 R:H<sub>2</sub>O, S:THF, heated

##### Notes

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

##### References

[Fabrication of organic thin-film transistors provided with polyacetylene semiconductor layers](#)

By Matsumoto, Shinji et al

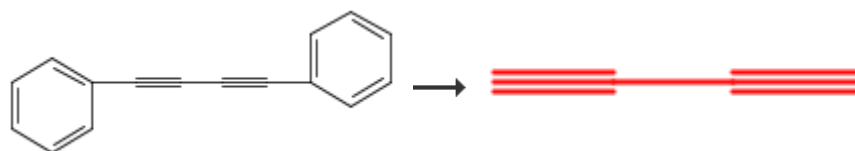
From Jpn. Kokai Tokkyo Koho, 2009224620, 01 Oct 2009

#### Experimental Procedure

Tetrahydrofuran solution of 10,12 pentacosadiynoic acid (manufactured by Tokyo Kasei Kogyo Co., Ltd.) (0.1 weight%) was developed in the silicon substrate with a thermally oxidized film (200nm), stored in a container filled with tetrahydrofuran steam. Then, subjected to heat treatment on a hot plate. A diacetylene monomer film was obtained.

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

#### 16. Single Step



### Overview

#### Steps/Stages

- 1.1 R:Me(CH<sub>2</sub>)<sub>11</sub>OSO<sub>3</sub>  
 - •Na<sup>+</sup>, R:Me(CH<sub>2</sub>)<sub>3</sub>CH<sub>2</sub>OH, R:NaCl, C:3524-62-7,  
 S:Cyclohexane, S:H<sub>2</sub>O, 12 h

#### Notes

photochemical, UV irradiation (365 nm) used,  
 Reactants: 1, Reagents: 3, Catalysts: 1,  
 Solvents: 2, Steps: 1, Stages: 1, Most stages  
 in any one step: 1

#### References

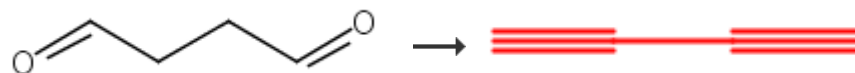
[Highly Swollen Liquid Crystals as New Reactors for the Synthesis of Nanomaterials](#)  
 By Surendran, Geetarani et al  
 From Chemistry of Materials, 17(6), 1505-1514; 2005

### Experimental Procedure

**Synthesis of Polymers.** The polymer samples were prepared as follows. For sample **4.A**, the solution was prepared by mixing 2 mL of an aqueous solution containing 0.0351 g of NaCl and 0.8 g of SDS with 5 mL of cyclohexane containing 0.19 g of 1,4-diphenylbutadiyne (Sigma Aldrich). The SLC was structured by the addition of 0.8 g of 1-pentanol under strong stirring. It was  $\gamma$  irradiated for 20 h, under nitrogen atmosphere (total amount of 90 kGy). The mesophase was further destabilized by the addition of 5 mL of ethanol and 5 mL of water. A phase separation occurs with the organic portion on the top containing the polymer. The polymer was recovered as a solid floating on water after full evaporation of the organic phase. Samples **4.B** and **4.C** were prepared according to the same process; sample **4.B** was prepared in pure cyclohexane, and sample **4.C** was prepared in the cyclohexane phase of the SLC. For sample **4.C**, the SLC was prepared as for sample **4.A**, but the organic phase was made of 3.8 g of cyclohexane, 0.38 g of 1,4-diphenylbutadiyne (Sigma Aldrich), and 0.193 g of benzene methyl ether (Fluka) used as a polymerization catalyst. The so-obtained SLC was left under UV irradiation (100 W, 365 nm) for 12 h. The polymer fibers were recovered according to the same process.

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

#### 17. Single Step



### Overview

#### Steps/Stages

- 1.1 C:Al<sub>2</sub>O<sub>3</sub>, 375°C; 375°C → 100°C; 100°C → 0°C; 0°C → -50°C

#### Notes

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

#### References

[Catalytic dehydration of acetaldehyde to produce ethyne](#)  
 By Everett, Christian  
 From U.S. Pat. Appl. Publ., 20040102647, 27  
 May 2004

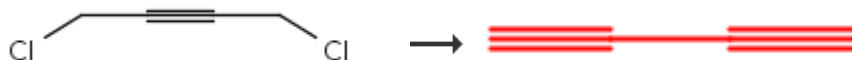
### Experimental Procedure



Succindialdehyde in the gas phase is passed through a reaction zone containing aluminum oxide at a temperature of 350 C. to produce diacetylene and water. The gas stream is cooled to 100 C. by passing through a cooling zone. The gas stream is then chilled to 10 C. causing the co-product water and unreacted or partially reacted succindialdehyde to liquify, whereby diacetylene is obtained as a gas. diacetylene

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 18. Single Step



#### Overview

#### Steps/Stages

1.1 R:KOH, S:H<sub>2</sub>O, S:THF

#### Notes

product typically generated immediately before use, Reactants: 1, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

#### References

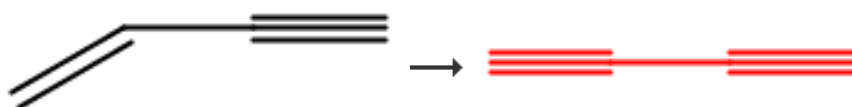
[Polyphospha\[m\]cyclo\[n\]carbons \(m+n = 15, 20, 25, 30, 40\)](#)

By Markl, Gottfried et al

From Chemistry - A European Journal, 6(20), 3806-3820; 2000

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 19. Single Step



#### Overview

#### Steps/Stages

1.1

#### Notes

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

#### References

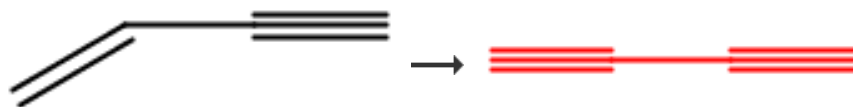
[Molecular dissociation of vinylacetylene and its implications for acetylene pyrolysis](#)

By Kiefer, John H. and Mitchell, Kevin I.

From Energy & Fuels, 2(4), 458-61; 1988

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 20. Single Step



[Overview](#)

**Steps/Stages**

1.1

**Notes**

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

**References**

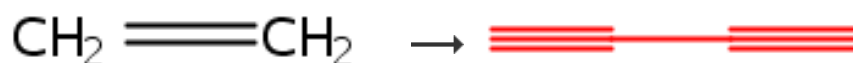
[Molecular dissociation of vinylacetylene and its implications for acetylene pyrolysis](#)

By Kiefer, John H. and Mitchell, Kevin I.

From Energy & Fuels, 2(4), 458-61; 1988

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**21. Single Step**



[Overview](#)

**Steps/Stages**

1.1

**Notes**

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

**References**

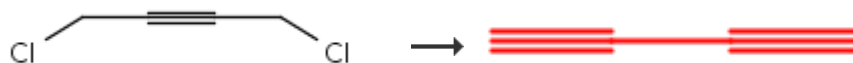
[Pyrolysis of methyl chloride, a pathway in the chlorine-catalyzed polymerization of methane](#)

By Weissman, Maia and Benson, Sydney W.

From International Journal of Chemical Kinetics, 16(4), 307-33; 1984

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**22. Single Step**



60%

[Overview](#)

**Steps/Stages**

**Notes**

1.1 S:H<sub>2</sub>O, S:Dioxane

Classification: Elimination;  
Dehydrochlorination; Isomerisation; #  
Conditions: KOH; H<sub>2</sub>O 1,4-dioxan; Rf,  
Reactants: 1, Solvents: 2, Steps: 1, Stages: 1,  
Most stages in any one step: 1

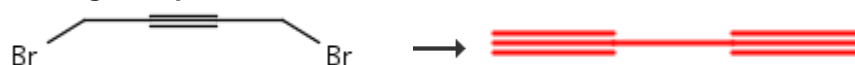
**References**

[Acetylenic compounds. XXVIII. A new route to diacetylene and its symmetrical derivatives](#)

By Armitage, J. B. et al

From Journal of the Chemical Society, , 44-7;  
1951

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**23. Single Step**[Overview](#)**Steps/Stages**1.1 R:NaNH<sub>2</sub>**Notes**

Classification: Elimination;  
Dehydrohalogenation; # Conditions: NaNH<sub>2</sub>; #  
Comments: generalized reaction, halogen can vary; other metal amides can be used,  
Reactants: 1, Reagents: 1, Steps: 1, Stages: 1,  
Most stages in any one step: 1

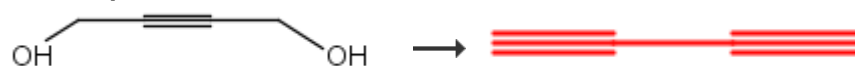
**References**

[The chemistry of the alkali amides. III](#)

By Levine, Robert and Fernelius, W. Conard

From Chemical Reviews (Washington, DC,  
United States), 54, 449-573; 1954

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**24. 2 Steps**[Overview](#)**Steps/Stages**1.1 R:SOCl<sub>2</sub>, R:C<sub>5</sub>H<sub>5</sub>N, cooled; 1 h, cooled; 20 h, cooled2.1 R:KOH, S:H<sub>2</sub>O, S:DMSO, rt → 75°C**Notes**

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

**References**

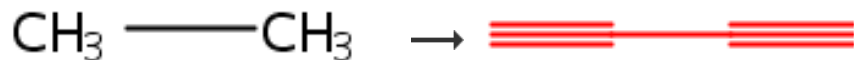
[Methods of preparing dicarbonyl compounds from biomass waste](#)

By Klein, Josef Peter

From PCT Int. Appl., 2015060862, 30 Apr  
2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 25. 2 Steps



#### Overview

#### Steps/Stages

- 1.1
- 2.1

#### Notes

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

#### References

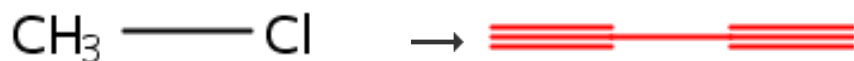
[Pyrolysis of methyl chloride, a pathway in the chlorine-catalyzed polymerization of methane](#)

By Weissman, Maia and Benson, Sydney W.

From International Journal of Chemical Kinetics, 16(4), 307-33; 1984

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 26. 2 Steps



#### Overview

#### Steps/Stages

- 1.1
- 2.1

#### Notes

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

#### References

[Pyrolysis of methyl chloride, a pathway in the chlorine-catalyzed polymerization of methane](#)

By Weissman, Maia and Benson, Sydney W.

From International Journal of Chemical Kinetics, 16(4), 307-33; 1984

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 27. 3 Steps



#### Overview

**Steps/Stages**

- 1.1 R:NaHCO<sub>3</sub>, C:1319-53-5, C:16753-36-9, S:H<sub>2</sub>O, 2 h, 90°C, 5 psi, pH 6
- 2.1 R:SOCl<sub>2</sub>, R:C<sub>5</sub>H<sub>5</sub>N, cooled; 1 h, cooled; 20 h, cooled
- 3.1 R:KOH, S:H<sub>2</sub>O, S:DMSO, rt → 75°C

**Notes**

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

**References**

[Methods of preparing dicarbonyl compounds from biomass waste](#)

By Klein, Josef Peter

From PCT Int. Appl., 2015060862, 30 Apr 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**28. 3 Steps**[Overview](#)**Steps/Stages**

- 1.1
- 2.1
- 3.1

**Notes**

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

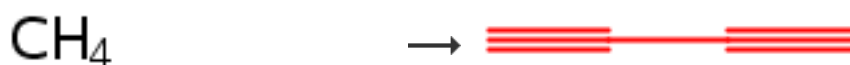
**References**

[Pyrolysis of methyl chloride, a pathway in the chlorine-catalyzed polymerization of methane](#)

By Weissman, Maia and Benson, Sydney W.

From International Journal of Chemical Kinetics, 16(4), 307-33; 1984

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**29. 3 Steps**[Overview](#)**Steps/Stages**

- 1.1
- 2.1
- 3.1

**Notes**

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

**References**

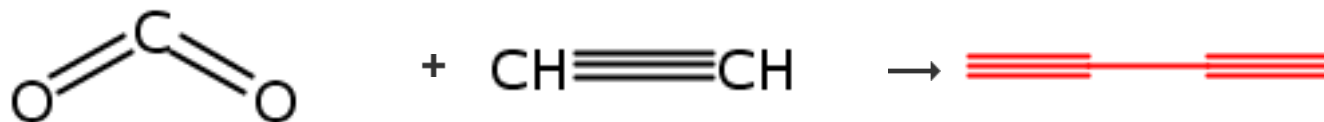
[Pyrolysis of methyl chloride, a pathway in the chlorine-catalyzed polymerization of methane](#)

By Weissman, Maia and Benson, Sydney W.

From International Journal of Chemical Kinetics, 16(4), 307-33; 1984

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 30. 4 Steps



[Step 2.1]

#### Overview

#### Steps/Stages

- 1.1 C:TiO<sub>2</sub>, S:H<sub>2</sub>O, > 1 h
- 2.1 R:NaHCO<sub>3</sub>, C:1319-53-5, C:16753-36-9, S:H<sub>2</sub>O, 2 h, 90°C, 5 psi, pH 6
- 3.1 R:SOCl<sub>2</sub>, R:C<sub>5</sub>H<sub>5</sub>N, cooled; 1 h, cooled; 20 h, cooled
- 4.1 R:KOH, S:H<sub>2</sub>O, S:DMSO, rt → 75°C

#### Notes

1) xenon or mercury lamp used, photochemical, Reactants: 2, Reagents: 4, Catalysts: 3, Solvents: 2, Steps: 4, Stages: 4, Most stages in any one step: 1

#### References

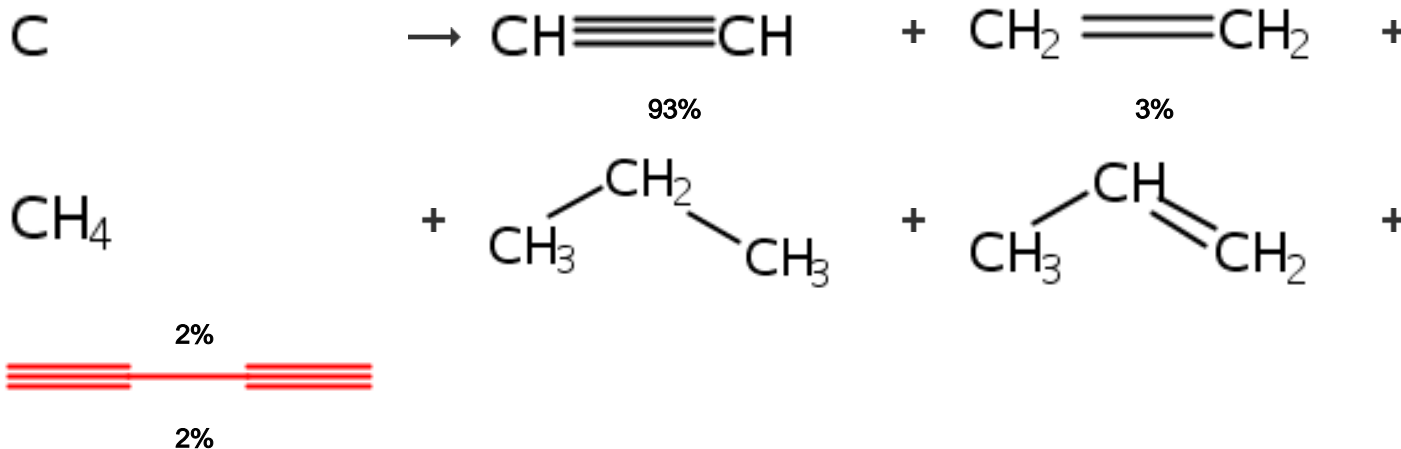
[Methods of preparing dicarbonyl compounds from biomass waste](#)

By Klein, Josef Peter

From PCT Int. Appl., 2015060862, 30 Apr 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 31. Single Step



#### Overview

#### Steps/Stages

#### Notes

1.1 R:H<sub>2</sub>, rt, 760 mmHg

photochemical, other products detected, ruby laser used, the product yields depend on hydrogen and argon pressure, gas phase, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

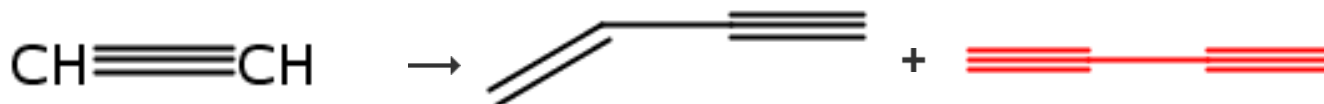
**References**

[Reactions of laser-generated carbon vapor with hydrogen](#)

By Quinn, John F.

From null, , 156 pp.; 1973

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

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

1.1 R:MeSSMe

**Notes**

thermal, other products also detected, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

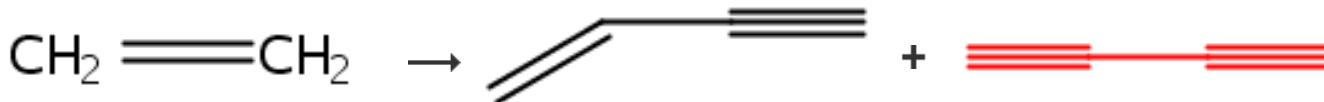
**References**

[Radical analysis in the pyrolysis of hydrocarbons by scavenging with dimethyl disulfide](#)

By Guthier, K. et al

From Berichte der Bunsen-Gesellschaft, 97(1), 140-2; 1993

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**33. 2 Steps**[Overview](#)**Steps/Stages****Notes**

1.1 R:MeSSMe

2.1 R:MeSSMe

1) thermal, other products also detected, 2) thermal, other products also detected,  
 Reactants: 1, Reagents: 1, Steps: 2, Stages: 2, Most stages in any one step: 1

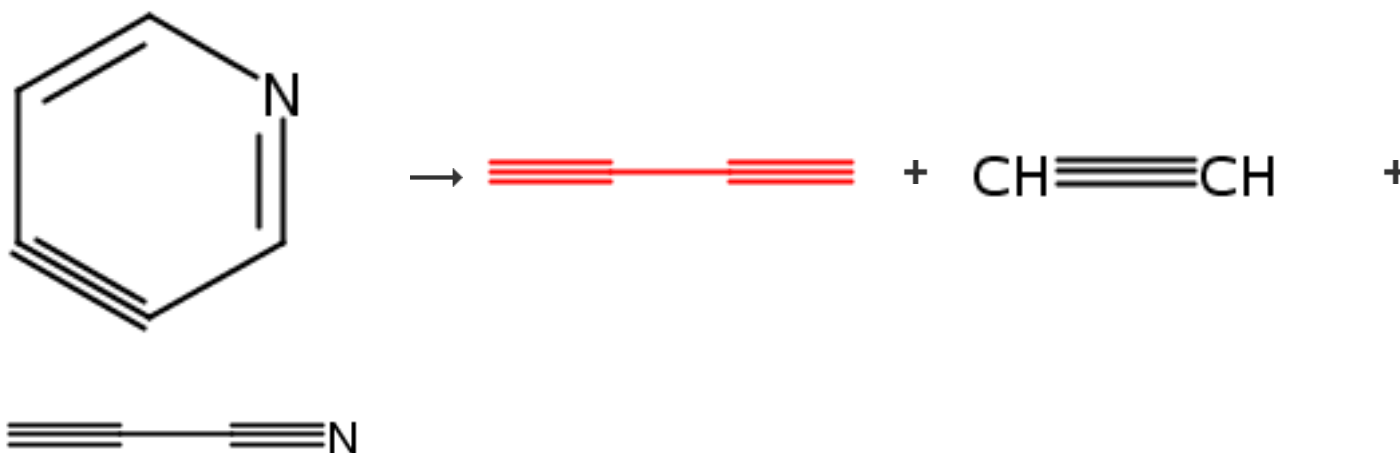
**References**

[Radical analysis in the pyrolysis of hydrocarbons by scavenging with dimethyl disulfide](#)

By Guthier, K. et al

From *Berichte der Bunsen-Gesellschaft*, 97(1), 140-2; 1993

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**34. Single Step**[Overview](#)**Steps/Stages**1.1 R:HCN, S:N<sub>2</sub>**Notes**

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

**References**

[First direct observation of pyridyne: matrix infrared study of the photolysis products of 3,4-pyridinedicarboxylic anhydride](#)

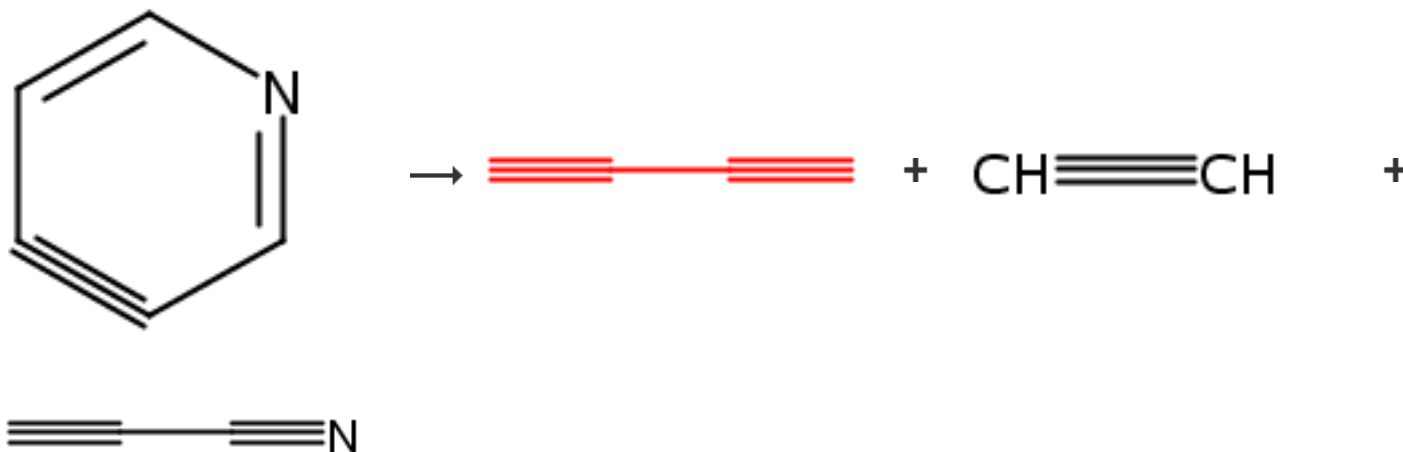
By Nam, H. H. and Leroi, G. E.

From *Journal of the American Chemical Society*, 110(12), 4096-7; 1988

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**35. Single Step**





### Overview

#### Steps/Stages

1.1 S:Ar

#### Notes

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

#### References

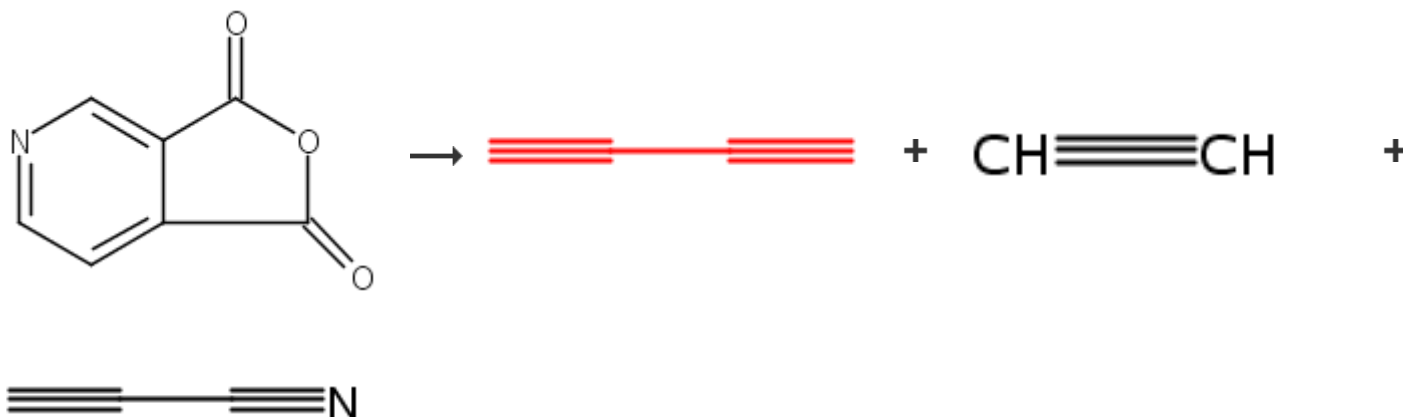
[First direct observation of pyridyne: matrix infrared study of the photolysis products of 3,4-pyridinedicarboxylic anhydride](#)

By Nam, H. H. and Leroi, G. E.

From Journal of the American Chemical Society, 110(12), 4096-7; 1988

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

#### 36. 2 Steps



### Overview

#### Steps/Stages

#### Notes

1.1 S:Ar  
2.1 S:Ar

1) photolysis  $\lambda > 340$  nm, 2) PHOTOCHEM.,  
Reactants: 1, Solvents: 1, Steps: 2, Stages: 2,  
Most stages in any one step: 1

### References

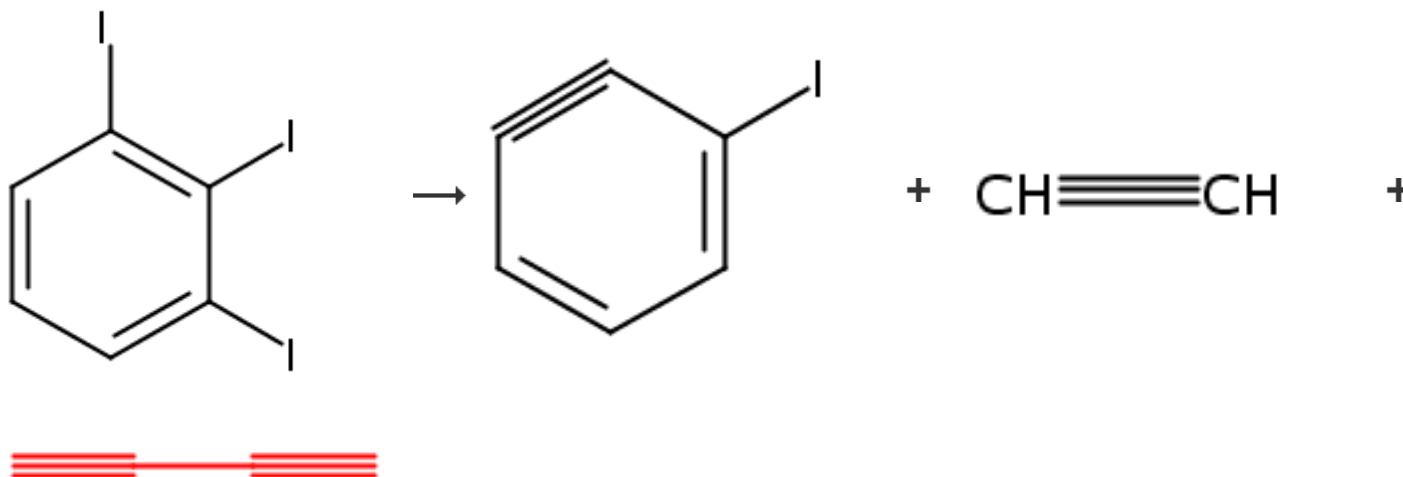
[First direct observation of pyridyne: matrix infrared study of the photolysis products of 3,4-pyridinedicarboxylic anhydride](#)

By Nam, H. H. and Leroi, G. E.

From Journal of the American Chemical Society, 110(12), 4096-7; 1988

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 37. Single Step



### Overview

#### Steps/Stages

1.1 690°C

### Notes

thermal, alternative preparation shown,  
Reactants: 1, Steps: 1, Stages: 1, Most stages  
in any one step: 1

### References

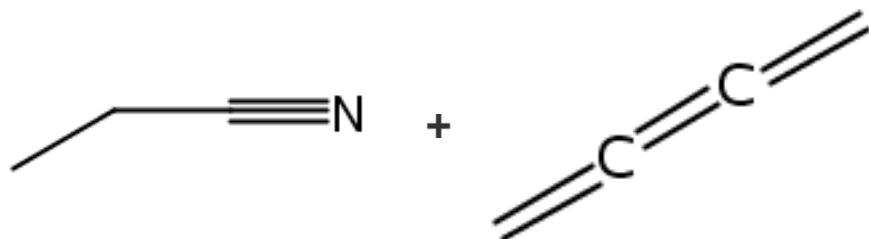
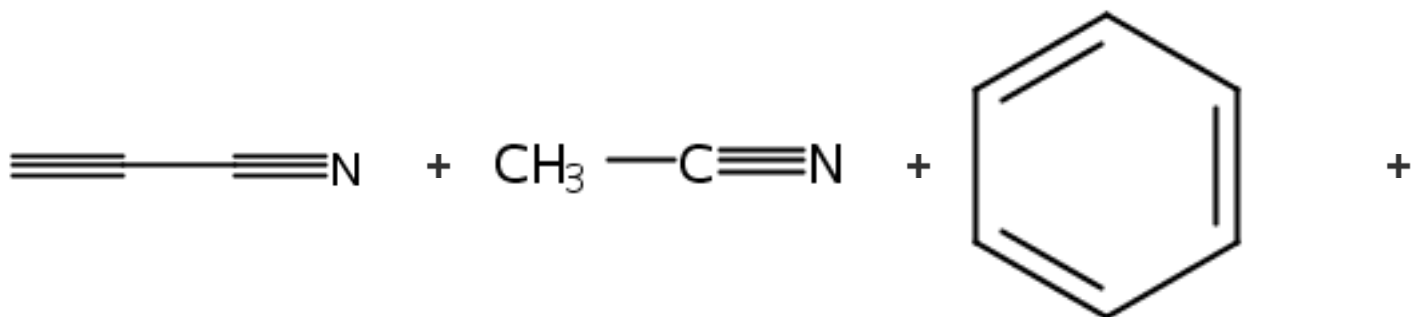
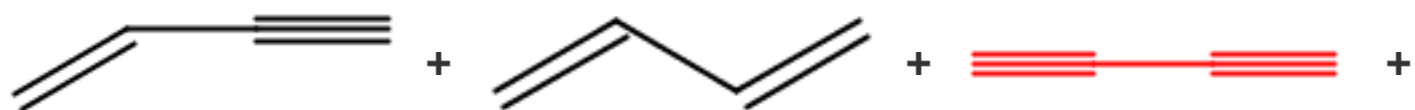
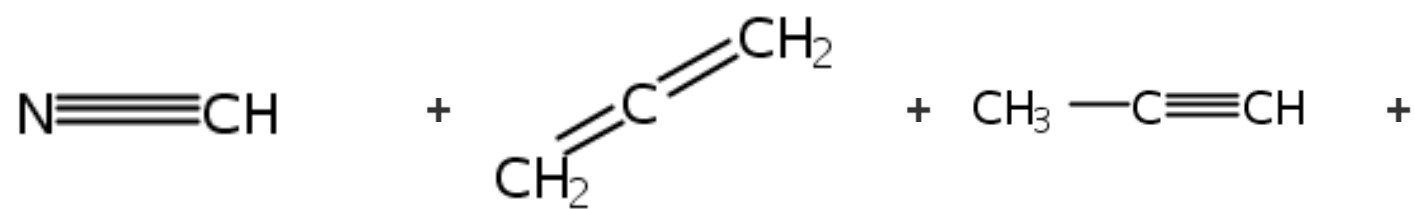
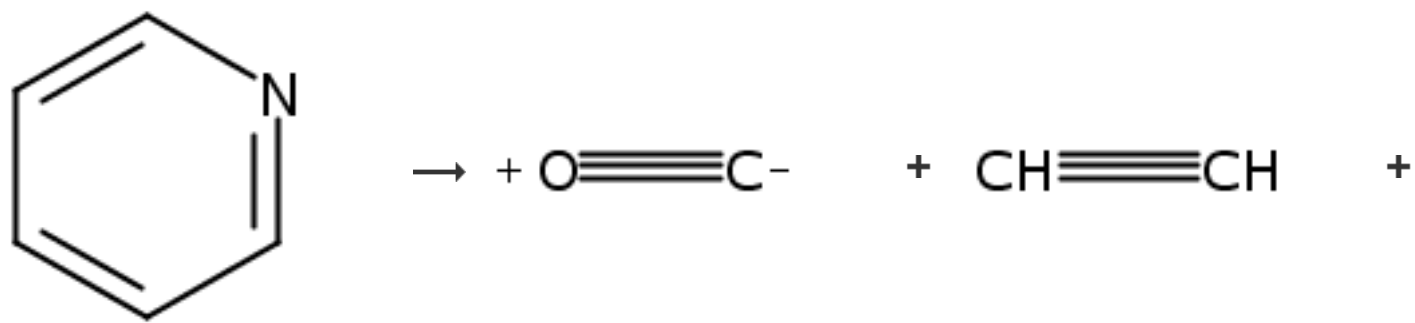
[1,2,3-Tridehydrobenzene](#)

By Venkataramani, Sugumar et al

From Angewandte Chemie, International Edition, 44(39), 6306-6311; 2005

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

### 38. Single Step



[Overview](#)

**Steps/Stages**

**Notes**

1.1 760 Torr

photochemical, gas phase, laser (260mJ at 193nm) irradiation, Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

[Laser Photochemical Etching of Silica: Nanodomains of Crystalline Chaoite and Silica in Amorphous C/Si/O/N Phase](#)

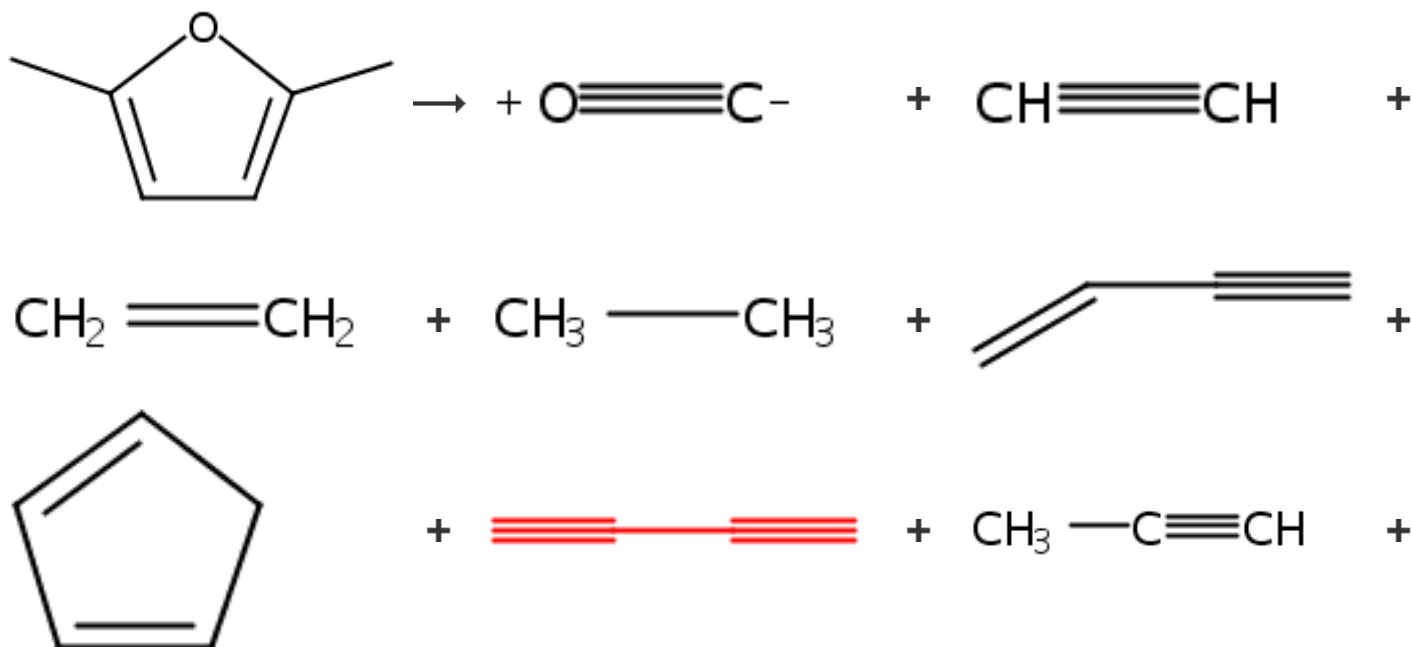
By Pola, Josef et al

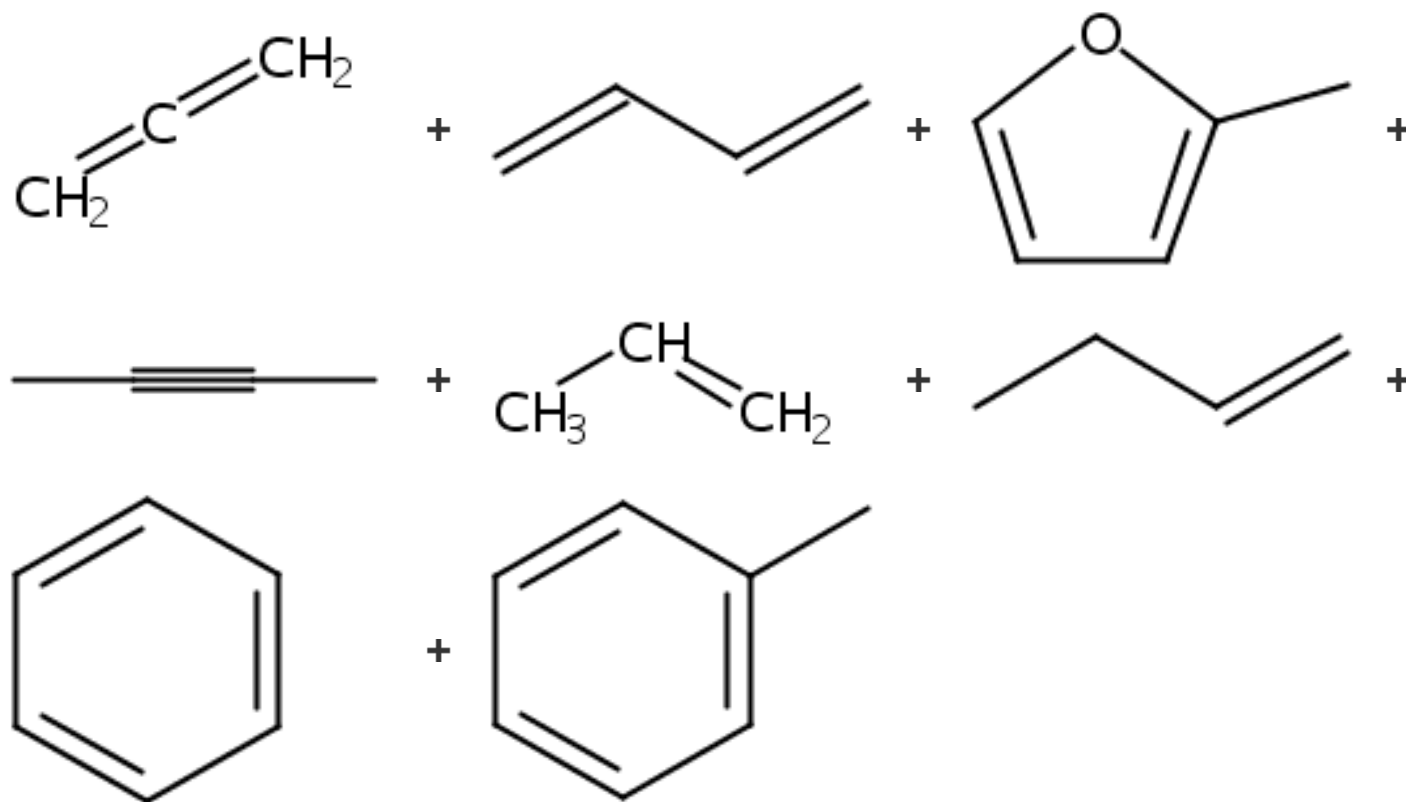
From Journal of Physical Chemistry C, 112(34), 13281-13286; 2008

**Experimental Procedure**

Laser irradiation experiments were conducted on gaseous pyridine (13 Torr) in helium (total pressure 760 Torr) admitted to a reactor (140 mL in volume) having two orthogonally positioned tubes: one furnished with UV-grade synthetic silica and the other with KBr windows. The reactor<sup>26</sup> had two side arms: one fitted with a rubber septum and the other connecting to a standard vacuum manifold. Pyridine samples were irradiated with an LPX 210i excimer (ArF) laser operating with a repetition frequency of 10 Hz. The laser pulses (fwhm 23 ns, 260 mJ at 193 nm) were focused to an incident area of 0.5 cm × 0.2 cm (fluence 2.6 J/cm<sup>2</sup>). This fluence corresponds to MW output and represents a critical threshold, as the described process does not occur at lower values. The progress of pyridine decomposition was monitored directly in the reactor by FTIR spectrometry (a Shimadzu FTIR IR Prestige-21 spectrometer) using diagnostic absorption of pyridine at 1590 cm<sup>-1</sup>. Aliquots of the irradiated reactor content were sampled by a gastight syringe (Dynatech Precision Sampling) and analyzed by gas chromatography-mass spectroscopy (a Shimadzu QP 5050 mass spectrometer (60 m capillary column Neutrabond-1, programmed temperature 30 - 200 °C)). The decomposition products were identified through their FTIR spectral diagnostic bands. Products- CO, C<sub>2</sub>H<sub>2</sub>, HCN, HC.ident.C-CN, HC.ident.C-C.ident.CH. (CO, 2130 and 2175 cm<sup>-1</sup>; C<sub>2</sub>H<sub>2</sub>, 731 cm<sup>-1</sup>; HCN, 713 cm<sup>-1</sup>; HC.ident.C-CN, 664 cm<sup>-1</sup>; HC.ident.C-C.ident.CH 627 cm<sup>-1</sup>) and through mass spectra using the NIST library.

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

**39. Single Step**



### Overview

#### Steps/Stages

1.1 393K, 8 bar

#### Notes

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

#### References

[A Single Pulse Shock Tube Study on the Pyrolysis of 2,5-Dimethylfuran](#)

By Schuler, Dominik F. et al

From Zeitschrift fuer Physikalische Chemie (Muenchen, Germany), 229(4), 529-548; 2015

CASREACT®: Copyright © 2016 American Chemical Society. All Rights Reserved. CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.