

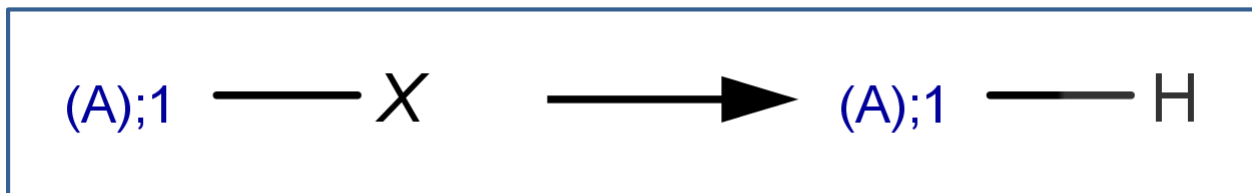
# Abiotic Reduction Reaction Library

Version 1.4 of the Abiotic Reduction Reaction Library contains eight reaction schemes:

- [Hydrogenolysis](#)
- [Vicinal Dehalogenation](#)
- [Nitroaromatic Reduction](#)
- [Aromatic Azo Reduction](#)
- [Sulfoxide Reduction](#)
- [N-Nitrosamine Reduction](#)
- [Quinone Reduction](#)
- [Isoxazole Cleavage](#)

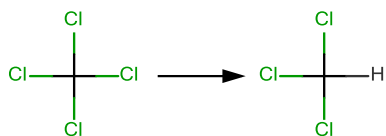
## Hydrogenolysis

SCHEME:

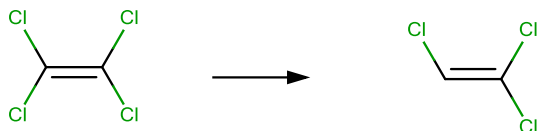


EXAMPLES:

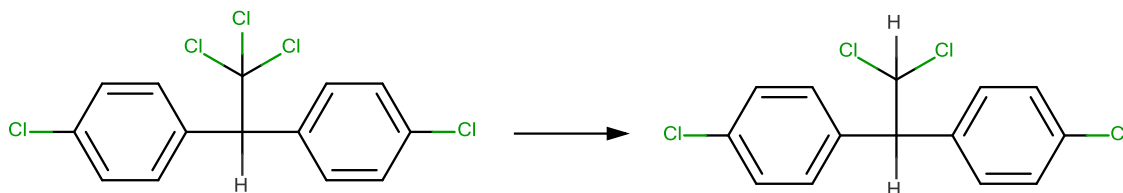
- Carbon tetrachloride (Elsner et al., 2004)



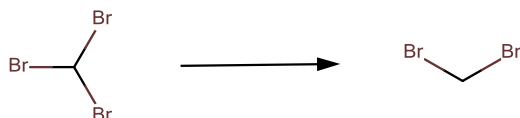
- Tetrachloroethene (Butler and Hayes, 1999)



- Dichlorodiphenyltrichloroethane (DDT) (Macalady et al., 1986; Larson and Weber, 1994)



- Tribromomethane (Perlinger et al., 1998)



## REFERENCES:

Elsner, M. et al. Mechanisms and Products of Surface-Mediated Reductive Dehalogenation of Carbon Tetrachloride by Fe(II) on Goethite. *Environ. Sci. Technol.* **2004**, *38*, 2058-2066.

Butler, E.C.; Hayes, K.F. Kinetics of the Transformation of Trichloroethylene and Tetrachloroethylene by Iron Sulfide. *Environ. Sci. Technol.* **1999**, *33*, 2021-2027.

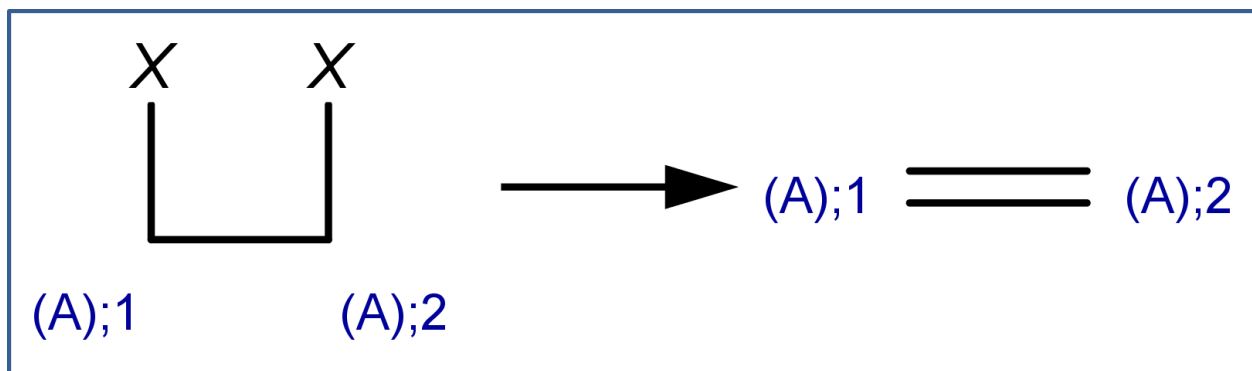
Macalady, D.L.; Tratnyek, P.G.; Grundl, T.J. Review Paper: Abiotic Reduction Reactions of Anthropogenic Organic Chemicals in Anaerobic Systems: A Critical Review. *J. Contam. Hydrol.* **1986**, *1*, 1-28.

Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

Perlinger, J.A.; Buschmann, J.; Angst, W.; Schwarzenbach, R.P. Iron Porphyrin and Mercaptojuglone Mediated Reduction of Polyhalogenated Methanes and Ethanes in Homogeneous Aqueous Solution. *Environ. Sci. Technol.* **1998**, *32*, 2431-2437.

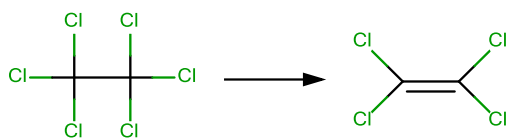
## Vicinal Dehalogenation

### SCHEME:

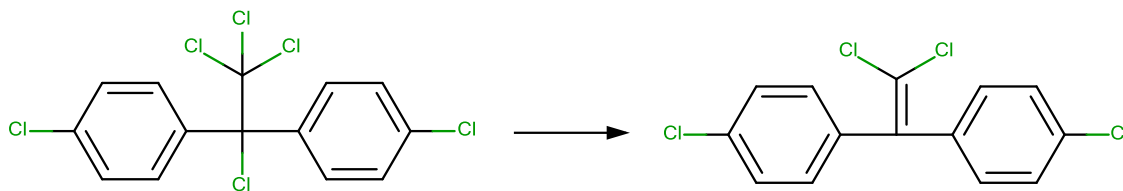


#### EXAMPLES:

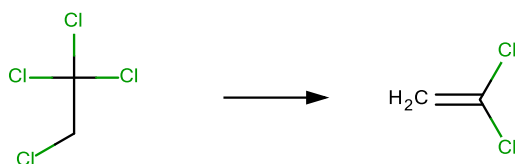
- Hexachloroethane (Perlinger et al., 1996)



- 1,1,1,2-tetrachloro-2,2-bis(p-chlorophenyl)ethane (Alpha-chloro-DDT, DTE) (Macalady et al., 1986; Larson and Weber, 1994)



- Tetrachloroethane (Butler and Hayes, 2000)



#### REFERENCES:

Perlinger, J.A.; Angst, W.; Schwarzenbach, R.P. Kinetics of the Reduction of Hexachloroethane by Juglone in Solutions Containing Hydrogen Sulfide. *Environ. Sci. Technol.* **1996**, *30*, 3408-3417.

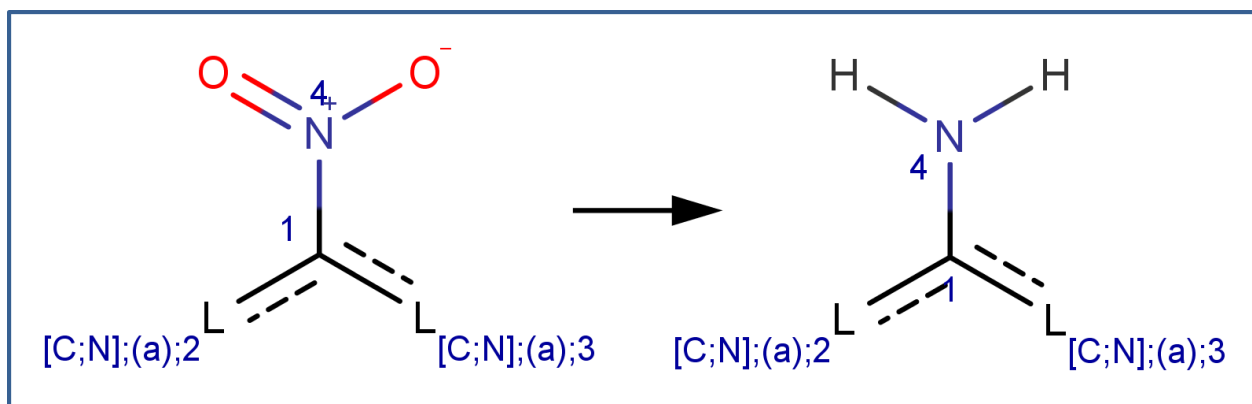
Macalady, D.L.; Tratnyek, P.G.; Grundl, T.J. Review Paper: Abiotic Reduction Reactions of Anthropogenic Organic Chemicals in Anaerobic Systems: A Critical Review. *J. Contam. Hydrol.* **1986**, *1*, 1-28.

Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

Butler, E.C.; Hayes, K.F. Kinetics of the Transformation of Halogenated Aliphatic Compounds by Iron Sulfide. *Environ. Sci. Technol.* **2000**, 34, 422-429.

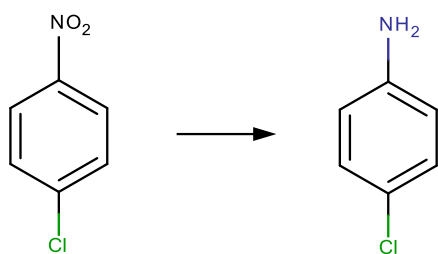
## Nitroaromatic Reduction

SCHEME:

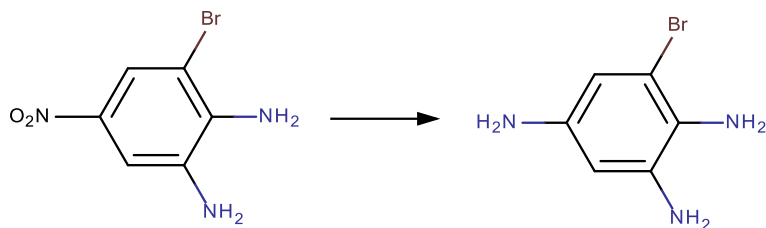


EXAMPLES:

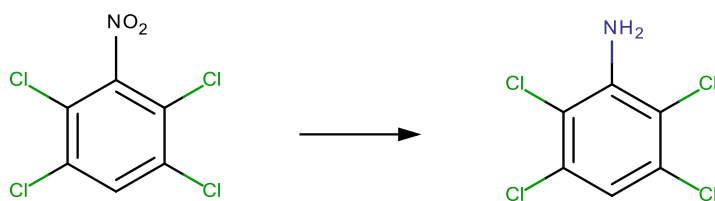
- P-Chloronitrobenzene (Klausen et al., 1995)



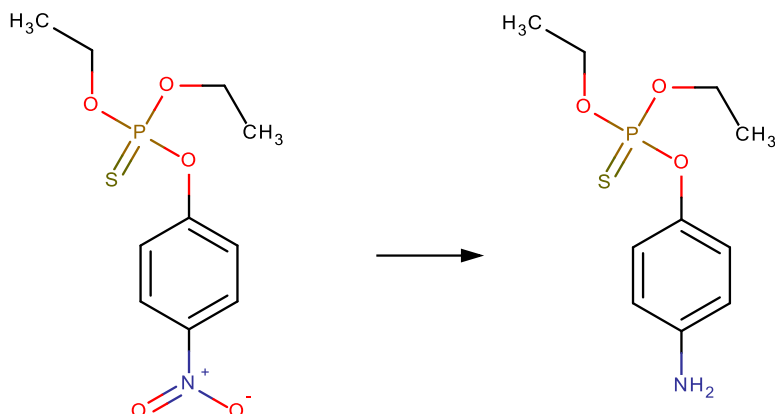
- 3-Bromo-5-nitrobenzene-1,2-diamine (Weber and Adams, 1995; Larson and Weber, 1994)



- 1,2,4,5-Tetrachloro-3-nitrobenzene (Macalady et al., 1986)



- O,O-diethyl O-4-nitrophenyl Phosphorothioate (Parathion) (Macalady et al., 1986)



## REFERENCES:

Klausen, J.; Trober, S.P.; Haderlein, S.B.; Schwarzenbach, R.P. Reduction of Substituted Nitrobenzenes by Fe(II) in Aqueous Mineral Suspensions. *Environ. Sci. Technol.* **1995**, *29*, 2396-2404.

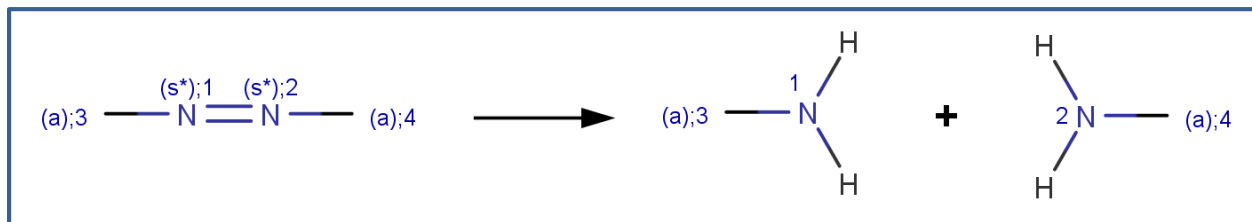
Weber, E.J.; Adams, R.L. Chemical- and Sediment-Mediated Reduction of the Azo Dye Disperse Blue 79. *Environ. Sci. Technol.* **1995**, *29*, 1163-1170.

Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

Macalady, D.L.; Tratnyek, P.G.; Grundl, T.J. Review Paper: Abiotic Reduction Reactions of Anthropogenic Organic Chemicals in Anaerobic Systems: A Critical Review. *J. Contam. Hydrol.* **1986**, *1*, 1-28.

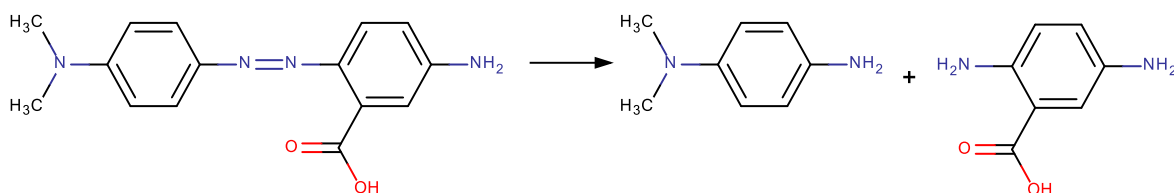
## Aromatic Azo Reduction

### SCHEME:

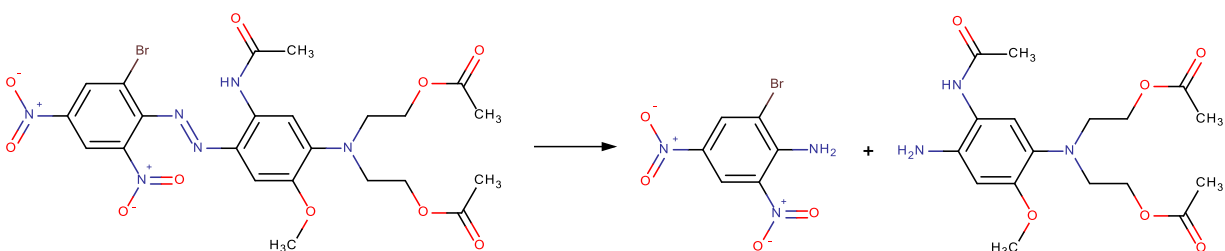


### EXAMPLES:

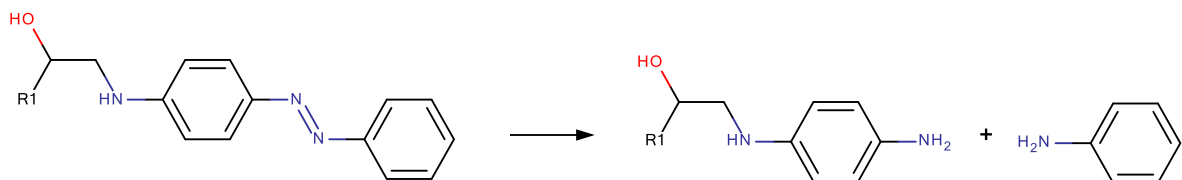
- 5-amino-2-{2-[4-(dimethylamino)phenyl]diazene-1-yl}benzoic acid (Weber and Wolfe, 1987)



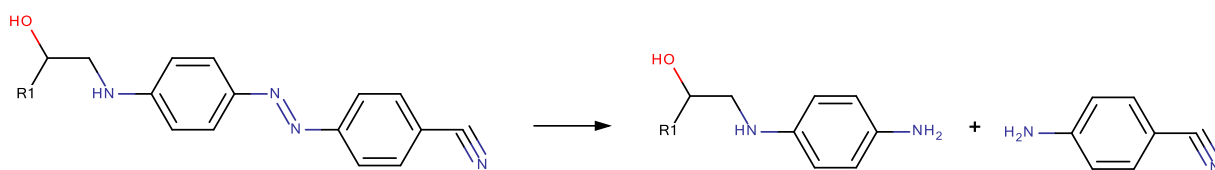
- Disperse Blue 79 (Weber and Adams, 1995; Larson and Weber, 1994)



- 1-({4-[(E)-2-phenyldiazene-1-yl]phenyl}amino)propan-2-ol (Substituted 4-Aminoazobenzene) (Weber, 1996)



- 4-[(E)-2-{4-[(2-hydroxypropyl)amino]phenyl}diazen-1-yl]benzonitrile (Substituted 4-cyano-4'-aminoazobenzene) (Zhang and Weber, 2009)



## REFERENCES:

Weber, E.J.; Wolfe, N.L. Kinetic Studies of the Reduction of Aromatic Azo Compounds in Anaerobic Sediment/Water Systems. *Environ. Toxicol. Chem.* **1987**, *6*, 911-919.

Weber, E.J.; Adams, R.L. Chemical- and Sediment-Mediated Reduction of the Azo Dye Disperse Blue 79. *Environ. Sci. Technol.* **1995**, *29*, 1163-1170.

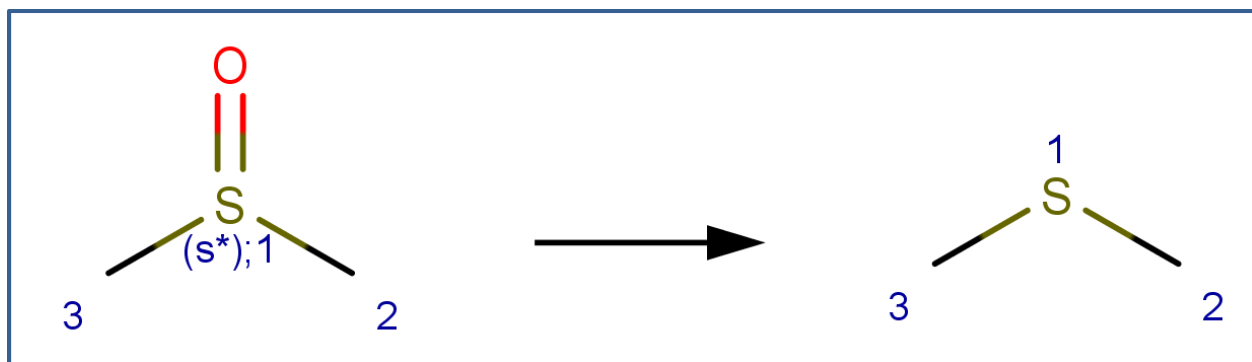
Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

Weber, E.J. Iron-Mediated Reductive Transformations: Investigation of Reaction Mechanism. *Environ. Sci. Technol.* **1996**, *30*, 716-719.

Zhang, H.; Weber, E.J. Elucidating the Role of Electron Shuttles in Reductive Transformations in Anaerobic Sediments. *Environ. Sci. Technol.* **2009**, *43*, 1042-1048.

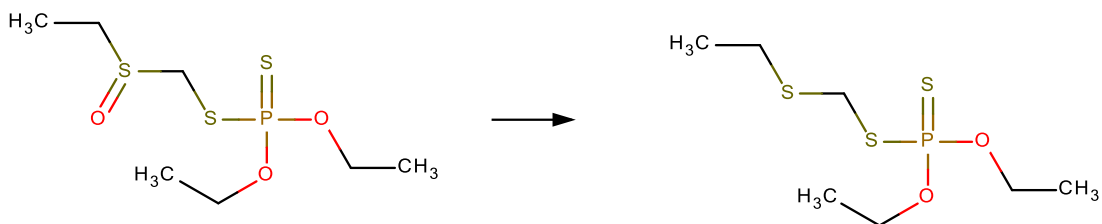
## Sulfoxide Reduction

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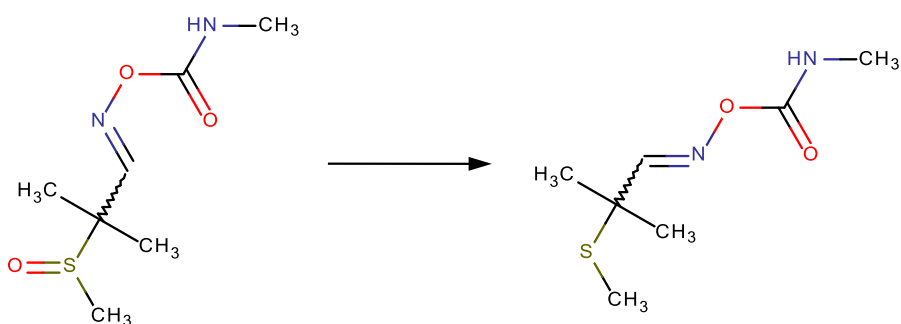


### EXAMPLES:

- Phorate Sulfoxide (Larson and Weber, 1994)



- Aldicarb Sulfoxide (Larson and Weber, 1994)

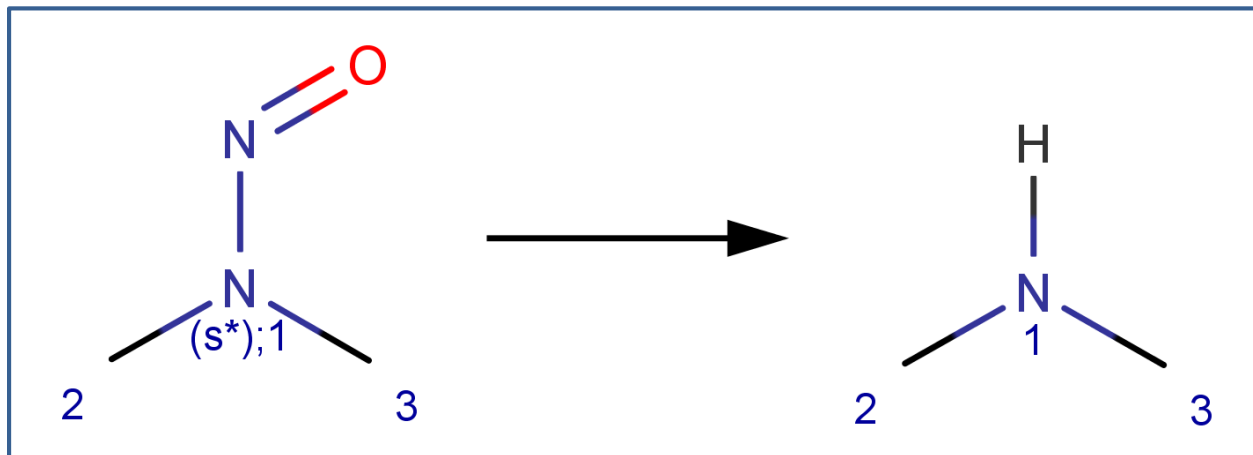


#### REFERENCES:

Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

## N-Nitrosoamine Reduction

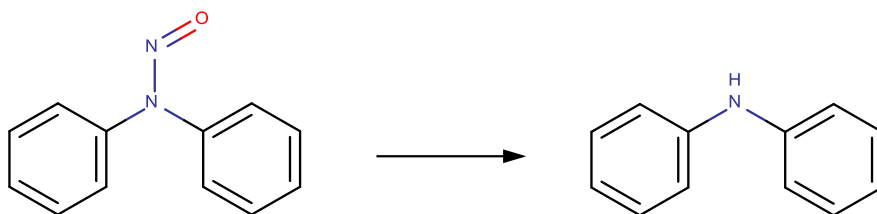
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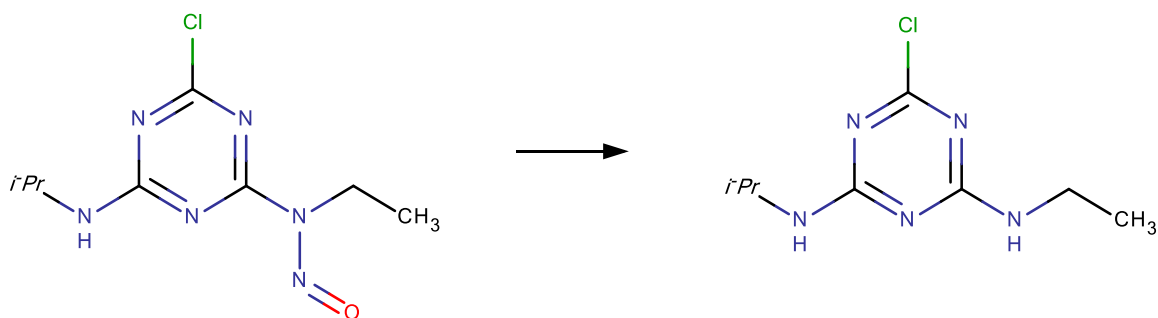


### EXAMPLES:

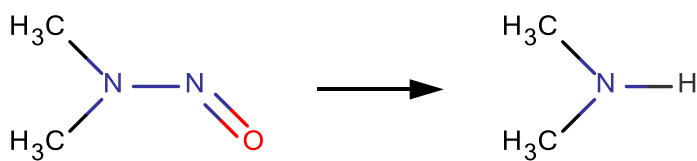
- Nitrosodiphenylamine (Larson and Weber, 1994)



- N-Nitrosoatrazine (Larson and Weber, 1994)



- Nitrosodimethylamine (Kulikova et al., 2009)



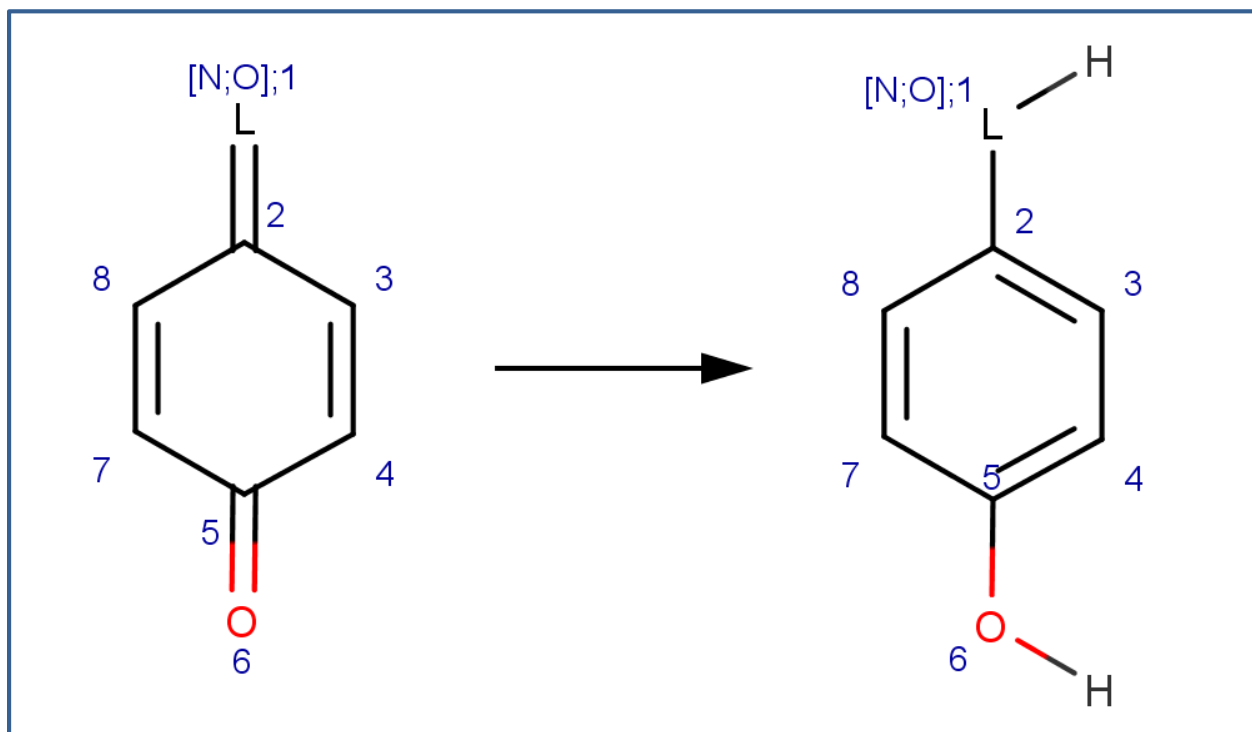
### REFERENCES:

Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

Kulikova, N.; Baker, M.; Gabryelski, W. Collision induced dissociation of protonated N-nitrosodimethylamine by ion trap mass spectrometry: Ultimate carcinogens in gas phase. *Int. J. Mass Spec.* **2009**, 288, 75-83.

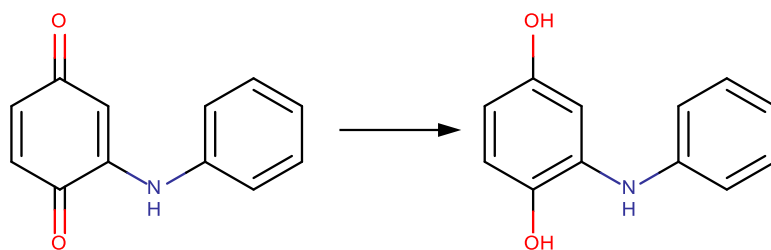
## Quinone Reduction

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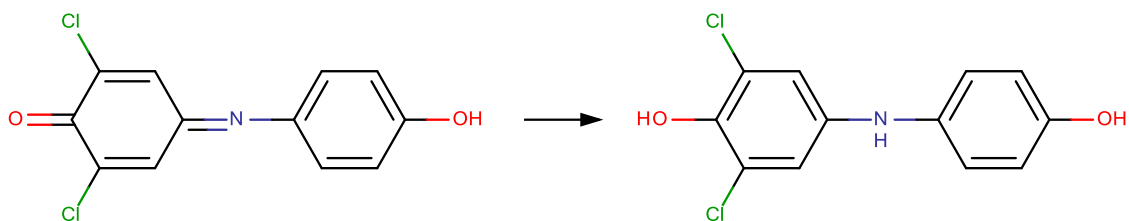


EXAMPLES:

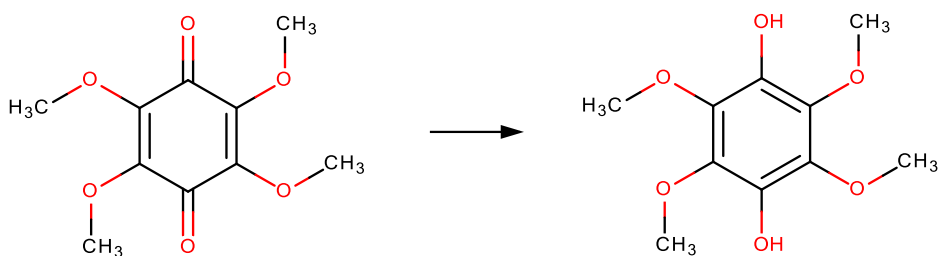
- Anilinohydroquinone (Colon et al., 2002)



- 2,6-dichlorophenolindophenol (Tonomura et al., 1978; Larson and Weber, 1994)



- Tetramethoxycyclohexa-2,5-diene-1,4-dione (Ref ??)



## REFERENCES:

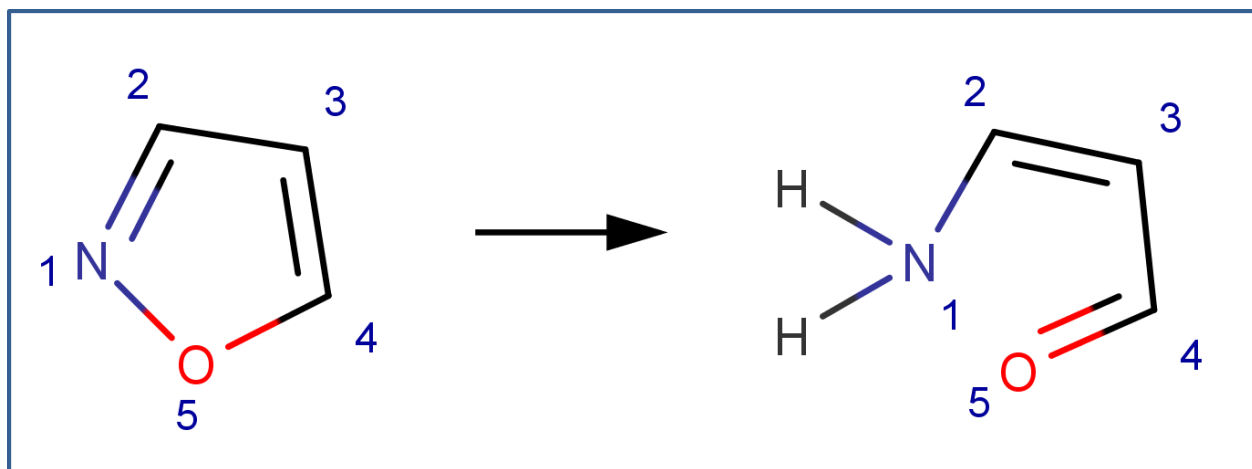
Colón, D.; Weber, E.J.; Baughman, G.L. Sediment-Associated Reactions of Aromatic Amines. 2. QSAR Development. *Environ. Sci. Technol.* **2002**, *36*, 2443-2450.

Tonomura, B.; Nakatani, H.; Ohnishi, M.; Yamaguchi-Ito, J.; Hiromi, K. Reduction for 2,6-Dichlorophenolindophenol and Potassium Ferricyanide by L-Ascorbic Acid. *Anal. Biochem.* **1978**, *84*, 370-383.

Larson, R.A. and E.J. Weber. *Reaction Mechanisms in Environmental Organic Chemistry*. Boca Raton: CRC Press, Inc., 1994.

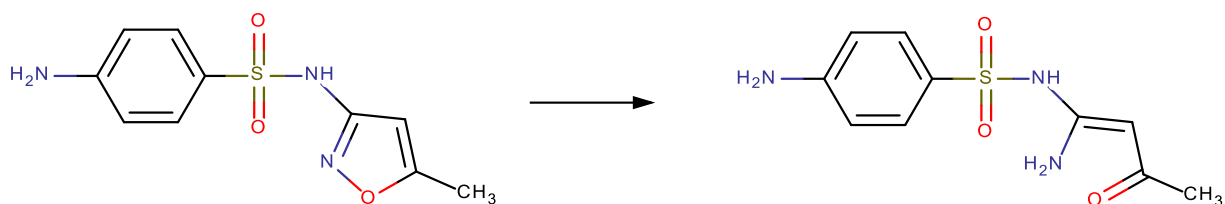
## Isoxazole Cleavage

### SCHEME:



#### EXAMPLES:

- Sulfamethoxazole (Mohatt et al., 2011)



#### REFERENCES:

Mohatt, J.L.; Hu, L.; Finneran, K.T.; Strathmann, T.J. Microbially Mediated Abiotic Transformation of the Antimicrobial Agent Sulfamethoxazole under Iron-Reducing Soil Conditions. *Environ. Sci. Technol.* **2011**, *45*, 4793-4801.