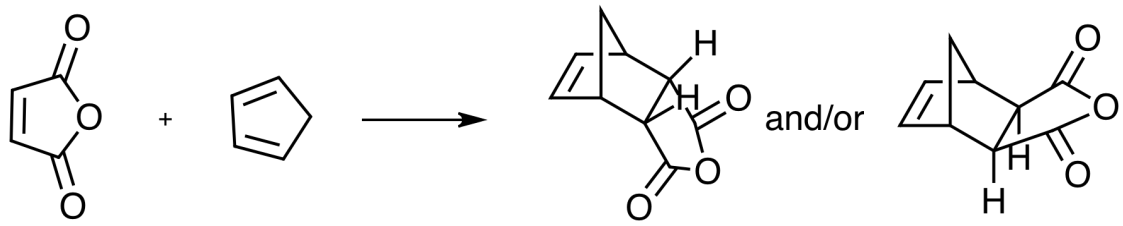
Diels-Alder

Summary:

The Diels-Alder reaction remains one of the most important reactions for constructing 6-membered rings, involving the reaction of a 1,3-diene with an alkene (dienophile). A traditional Diels-Alder reaction involves a simple diene such as 1,3-cyclopentadiene and maleic anhydride. The reaction proceeds by the thermal decomposition of dicyclopentadiene.



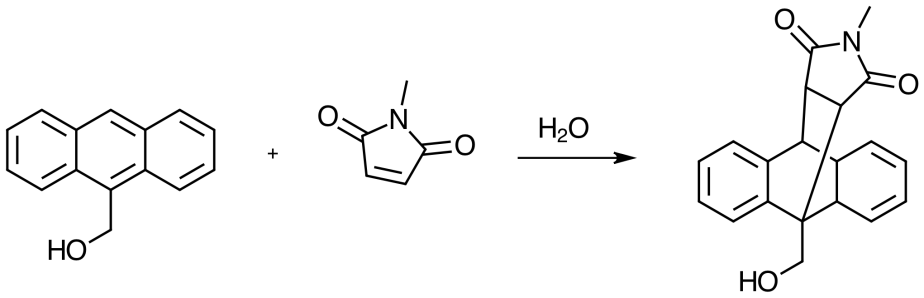
Reference: Reaction of 1,3-cyclopentadiene and maleic anhydride, Experimental Organic Chemistry, 5th Edition, Gilbert and Martin, 2011, p. 429-430

Chemical Name Aldrich Catalog #	Amount per 100 students (g or mL)	EH&S	Purchasing cost per 100 students ($)
Dicyclopentadiene 454338	345 g		$23.74
Maleic anhydride M188	5 g		$0.25
Ethyl acetate 270989	20 mL		$0.82
Petroleum ether 320447	20 mL	*F	$1.38
Calcium chloride, anhyd. 793639	25 g		$10.55

Diels-Alder: A Greener Approach

Summary:

This Diels-Alder reaction is performed in water and eliminates the requirement to prepare the starting material (thermal decomposition is required in the traditional approach). This approach takes advantage of the hydrophobic effect, which increases the reaction rate.



Reference: Greener Solutions for the Organic Chemistry Teaching Lab: Exploring the Advantages of Alternative Reaction Media, McKenzie, L.C., Huffman, L.M., Hutchison, J.E., Rogers, C.E., Goodwin, T.E., Spessard, G.O., J. Chem. Educ. 2009, 86, 488–493

Chemical Name Aldrich Catalog #	Amount per 100 students (g or mL)	EH&S	Purchasing cost per 100 students ($)
9-Anthracenemethanol 187240	3.25 g		$20.12
N-methylmaleimide 389412	5.2 g		$33.70
Water n/a	2500 mL		n/a

Comparison: Diels-Alder

Comparison of greener and traditional lab:

- Greener method uses water as a solvent and eliminates the need for hazardous organic solvents

	Purchasing costs	Waste reduction (per 100 students)	"Greener" benefits
Greener method	$53.82	2.5L aqueous waste	
Traditional method	$60.73	390 mL liquid waste 25 g solid waste	

Other greener lab options to explore:

- Diels–Alder Cycloadditions: A MORE Experiment in the Organic Laboratory Including A Diene Identification Exercise Involving NMR Spectroscopy and Molecular Modeling, J. Chem. Educ., 2005, 82 (4), p 625
- Microwave-Enhanced Organic Syntheses for the Undergraduate Laboratory: Diels−Alder Cycloaddition, Wittig Reaction, and Williamson Ether Synthesis, J. Chem. Educ., 2010, 87 (1), pp 84–86
- Microwave-Assisted Synthesis of a Natural Insecticide on Basic Montmorillonite K10 Clay. Green Chemistry in the Undergraduate Organic Laboratory, J. Chem. Educ. 2006, 83, 270–272 (hetero)