

Diels-alder reaction:
synthesis of cis-
norbornene-5,6-endo-
dicarboxylic
anhydrid...



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Ronak Parikh U30682934 Experiment 2: Diels-Alder Reaction: Synthesis of cis-Norbornene-5, 6-endo-dicarboxylic anhydride Introduction: The main goal of this experiment is to perform a Diels-Alder reaction between 2, 3-dimethyl-1, 3-butadiene and maleic anhydride, identify the product and hydrolyze to form the dicarboxylic acid. Diels alder reactions are classified as pericyclic reaction, which is a reaction which involves a cyclic rearrangement of bonding electrons, which means that the bonds are broken and reformed instantaneously.

The reaction takes place in a single step without the use of intermediates, which is what makes this reaction stereospecific because substituent's never have a chance to " change around". When the experiment is complete a colorless platelike crystal will be formed and then they will be compared against the expected values. The melting point range that is found for the resulting crystals will show if a successful product resulted. Background Cyclopentadiene is universally used in Diels-Alder reactions and is stable dimer, dicyclopentadiene, which is the Diels-Alder adduct from two molecules of the diene.

Because a bottle of cyclopentadiene actually contains the dimer, it must be converted into the monomer prior to using it as a reactant. Making cyclopentadiene by heating and distillation of the dimer makes it a reverse Diels-Alder reaction. If the initial process of heating and distilling does not yield enough pure cyclopentadiene then a stock solution prepared by the lab staff can be used to continue the experiment. Mechan Cyclopentadiene Maleic Anhydride cis-Norbornene-5, 6-endo-dicarboxylic anhydride Diene Dienophile Diels-Alder Product Side Reaction

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The side reaction which occurs during the production of cis-Norbornene-5, 6-endo-dicarboxylic anhydride is the dimerization of the diene. The remedy for this side reaction is to distill cyclopentadiene. Data Weight of cis-Norbornene-5, 6-endo-dicarboxylic anhydride obtained = 0.295 g Percent Yield of cis-Norbornene-5, 6-endo-dicarboxylic anhydride = (Actual / Theoretical) * 100 Theoretical = (Cyclopentadiene g/MW of Cyclopentadiene) * (1 mol Cyclopentadiene / 1 mol cis-Norbornene-5, 6-endo-dicarboxylic anhydride) * (MW of cis-Norbornene-5, 6-endo-dicarboxylic anhydride) = (0.160 g / 6.10 g/mol) * (1/1) * (164.16g/mol) = .397 g Norbene % yield = (0.295 g / .397. g) * 100 = 74.3% Melting point of camphor obtained = 1580C ??? 1600C Discussion: Diels-Alder reactions have a unique type of stereoselectivity which is seen when a diene is cyclic. In the reaction of maleic anhydride with cyclopentadiene, for example, the endo isomer is formed (the substituents from the dienophile point to the larger) instead of the the exo isomer (the substituents from the dienophile point away from the larger). The preference for endo??? stereochemistry is "observed" in most Diels-Alder reactions.

The more hindered endo product is formed and understood by using molecular orbital theory to explain that overlap of the p orbitals on the substituent's on the dienophile with p orbitals on the diene is favorable, helping to bring the two molecules together. Often times, even though the endo product is formed initially, an exo isomer will be isolated from a Diels-Alder reaction. This occurs because the exo isomer, having less of steric strain than the Endo, is more stable, and because the Diels-Alder reaction is often reversible under the reaction conditions.

The Diels-Alder reaction also exhibits another form of stereoselectivity. Note that the diene and dienophile approach each other in parallel planes: the diene undergoes a syn addition to the dienophile. Therefore, groups that are cis in the dienophile are also cis in the product. The experiment yielded a positive result, with formation of the white plate like crystal. The crystal had melting point 158-160 Degrees which is close to the literature Value. This slight difference in melting points can be attributed to a small amount of impurities. This could be due to human error.