

FOSSEE Summer Fellowship 2022

Visualization of Diels-Alder Reaction

Using Jmol

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Submitted by

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I would like to thank my parents and family members for supporting me during my Internship and also I would like to thank each and every person who has helped me directly or indirectly during the internship.

With Regards,

Tahirali Chaudhary

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TABLE OF CONTENTS

1. Introduction.....	3
1.1 General description.....	6
1.2 The Diene.....	8
1.3 The Dienophile.....	9
2. Stereochemistry: stereospecificity of the reaction.....	10
2.1 Stereochemistry of Dienophiles.....	10
2.2 Stereochemistry of Dienes.....	13
3. The Endo-rule for Diels Alder reaction.....	16
4. Frontier orbital description of cycloadditions.....	18
5. Intramolecular Diels–Alder reaction.....	21
6. Dimerization of dienes by cycloaddition reactions.....	24
7. Regioselectivity in Diels Alder reaction.....	25
8. The Woodward–Hoffmann description of the Diels–Alder reaction.....	26
9. Conclusion.....	29
10. Script.....	29
11. References.....	36

Aim: To visualize the 3D models and study the stereochemistry of reactants, transition states and products in Diels alder reaction using Jmol.

Tools: Jmol version 14.32.39

1. Introduction

The Jmol is the open-source software which can provide a platform to understand the stereochemistry of the molecule by three-dimensional visualization and by making the animation of the reaction. The visualization of 3d orbitals in the molecule will be used to understand the Diels alder reaction through frontier orbital descriptors and Woodward-Hofmann rules. The jmol program is applicable to understand the various aspects of the Diels alder reaction which will be further discussed. The Jmol has many other features like bond length measurement, simulated NMR spectrum and loading of a pdb file from the database to study drug protein interaction etc. By using the Jmol one can explain the concepts of chemistry in a very easy way .

The procedure to use the Jmol is shown as below:

1. Open the **Jmol Version 14.32.39**

2. Select the **Model kit** from the **Toolbar**, select the **Carbon** atom and make the six-carbon chain.
3. Select the **Drag to Bond** Option from the **Model kit** and put the cursor on one terminal carbon and drag the cursor by right clicking to another terminal atom which forms the Cyclohexane.
4. Now Select the **Delete Bond** option in the **Model Kit** and delete two sigma bonds from the Cyclohexane and then add the double bonds in diene & dienophile by clicking in between the two atoms and make the substrate as required for the reaction.
5. Select the **Oxygen atom** from the **Model Kit** and make the carbonyl group in dienophile.

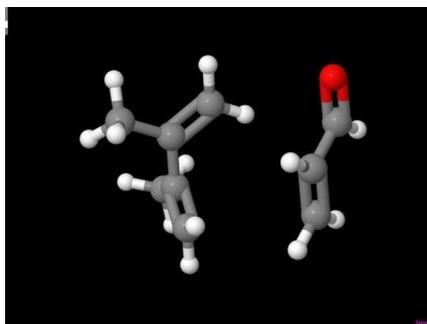


image 1.01

6. Now select the **SELECT** option from the **Toolbar** and select the 6 sp² hybridized carbon which we have to be labeled.
7. Now select the **Label** option from the **Display** option from the above and further select the **NAME** which will show the labels on the selected atoms.

8. Now Open the New file and make the Benzene ring and then after make the adduct as by same procedure as shown above to make molecule.

9. Now open the pop-up menu and select the none in select option and now click on select option given above in Jmol and select the 4 atoms in between which new sigma bond has formed by reaction and now change the bond colors from the pop-up menu and by same procedure change the color of the pi-bond also so from which can be identified that that are the newly formed bond.

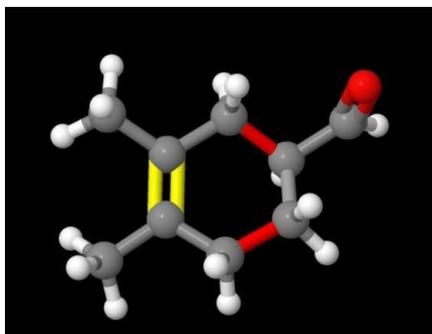


image 1.02

We can also use the script commands to use various features of the jmol so to enter the script command you have to open the console, select the file option and select the console to open the console.

Here there are some commands which are used in this project:

1. Connect: This can be used to show the forming and breaking of the bond in the molecule.

The general syntax is as follows:

connect [minimum and maximum distances] [source and target atom sets] [bond type] [radius option] [color option] [modify/create option]

2. Capture: This command can be used to save the animation in the device.

The general syntax is as follows:

```
capture "filename" (decimal)
```

3. Delete: This command will be used to delete the object

The general syntax is as follows:

```
delete $ [object id]
```

4. Draw: This command will be used to draw arrows, lines etc.

The general syntax is as follows:

```
draw [objectID] [modifying parameters] [positions]
```

5. LcaoCartoon: This command will be used to add orbitals

The general syntax is as follows:

```
lcaoCartoon CREATE "[type]"
```

6. Translate: This command will be used to adjust the molecule position

The general syntax is as follows:

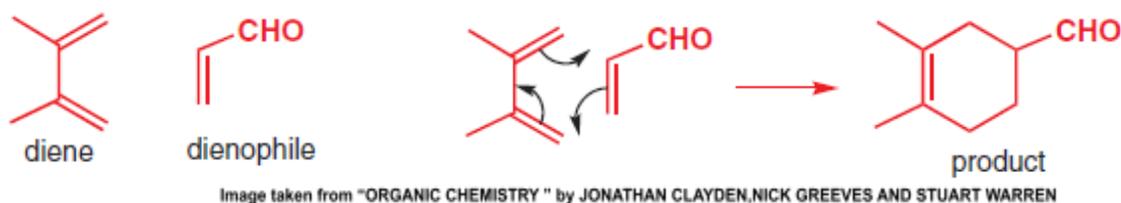
```
translate selected
```

Thus, by using this type of commands you can use the jmol for the visualization of the various react

1.1 General Description:

The Diels alder reaction is one of the best examples of the [4+2] Cycloaddition reaction. This reaction occurs between dialkenes and alkenes generally known as dienes and dienophiles respectively.

Here in the given example **2,3 methyl 1,3 butadiene** acts as a diene and **2-propenal** acts as a dienophile and both the molecule will react as a cycloaddition as shown in reaction to give a 6 membered cyclic product. The p-orbital of the double bond of the dienophile will overlap with the p-orbital of the sp² hybridized terminal carbon of the diene which results in the new sigma bond and similarly another terminal carbon of the diene will form a new sigma bond with dienophile as shown in figure. The double bond is shifted to the 2,3 position of the diene as shown in the **figure 1.1** the cyclic shifting of the bonds will appear.



1.1

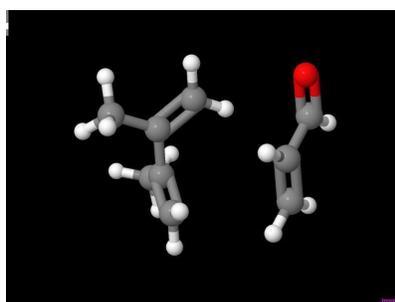


Image 1.11 (Substrate)

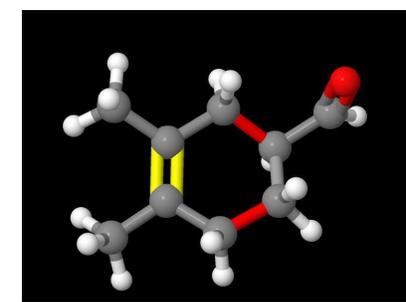
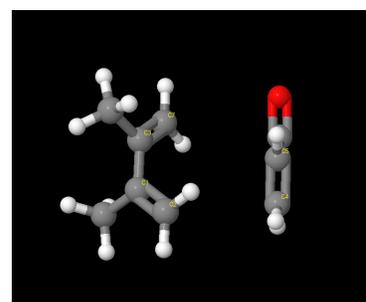


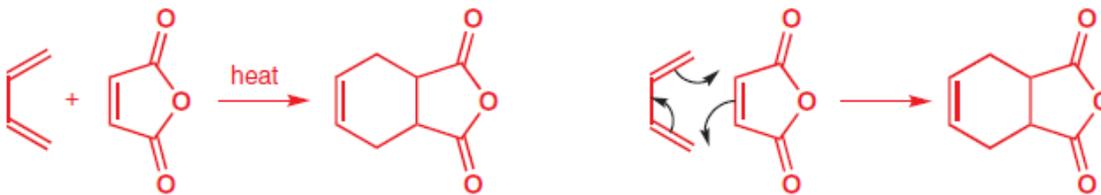
Image 1.12 (Product)



GIF 1.11

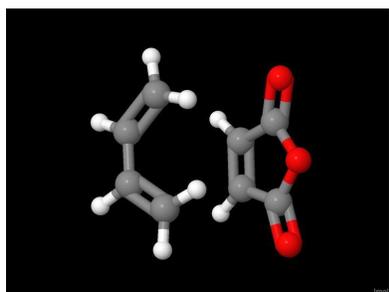
When the 1,3 butadiene reacts with Maleic anhydride it will give bicyclic product as shown in the reaction.

¹ #Gif 1.11 <https://drive.google.com/file/d/1ZHKGmf2EWajwW1eG25a97I5LpzyR4fZ/view?usp=sharing>



1.2

Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN



² Image 1.13 (Substrate)

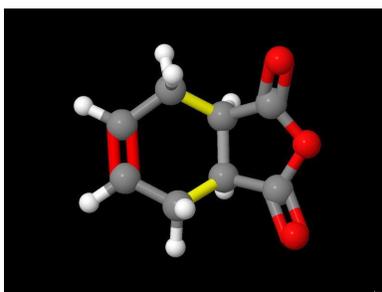
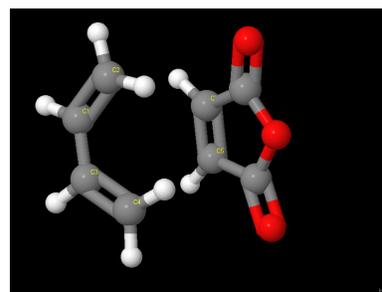


Image 1.14 (Product)

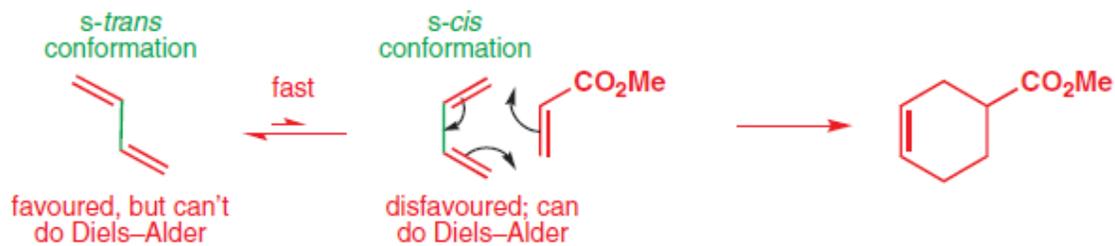


GIF 1.12

1.2 The Diene:

The diene in the Diels–Alder reaction will be in open-chain or cyclic form and it can also have various substituents. In the above example the Butadiene is taken as a diene and it can exist in two forms i.e., **Cis and Trans**, Usually the butadiene will be in the **Trans** conformation due to the Steric reasons. Although the **Cis** conformation is less stable, but it is favorable for this reaction so **Cis** conformation will take part in reaction because the rotation barrier between the **Cis and Trans** conformation is very less (i.e., 30 KJ mole⁻¹ at RT).

² Gif 1.12 <https://drive.google.com/file/d/1Rj6oztiXij1fEk6dSbh8c-Cy3z-N0kg/view?usp=sharing>



1.21

Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

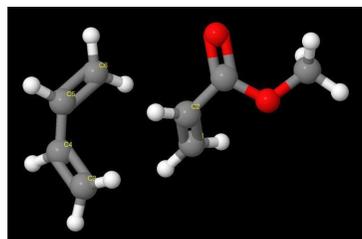


Image 1.21 (Substrate)

34

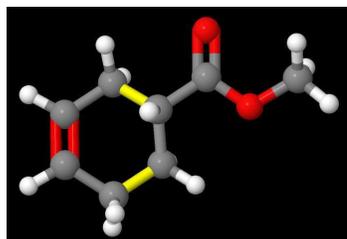
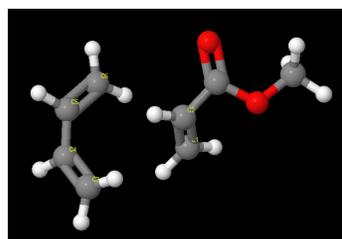
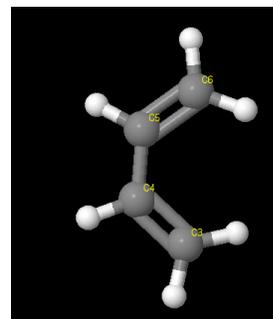


Image 1.22 (Product)



GIF 1.21



GIF 1.22

It can be concluded that **Cis** conformation is required for Diels alder reaction and molecules with **permanent Trans** confirmation cannot be able to participate in this reaction.

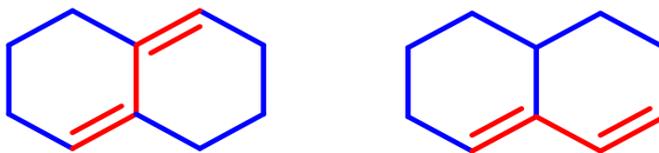


Image taken from slides provided by Prof. Krishna P Kaliappan

1.22

³ Gif 1.22 <https://drive.google.com/file/d/1ljIKMBeaQxLtrrgSBOIX-d43z1YP5CgV/view?usp=sharing>

⁴ Gif 1.21 <https://drive.google.com/file/d/13rsf1rvNveqhaszlrWldIoxRSKiNtLqs/view?usp=sharing>

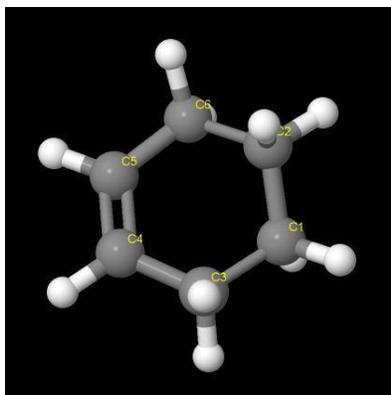
1.3 The Dienophile

The dienophiles should have an **electron-withdrawing group** conjugated to the alkene otherwise the reaction doesn't proceed or gives very poor yield. The simple reaction between butadiene and ethylene will give very poor yield because the electron-withdrawing group increases the reactivity of the dienophile. Hence if there is no electron-withdrawing group at the Dienophile as in below given example, the reaction will give poor yield due to less reactive dienophile.



Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

1.31



5

Image 1.32 (Product)

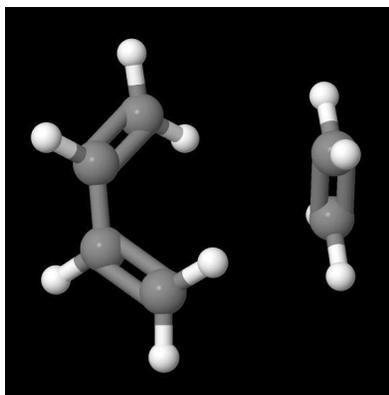
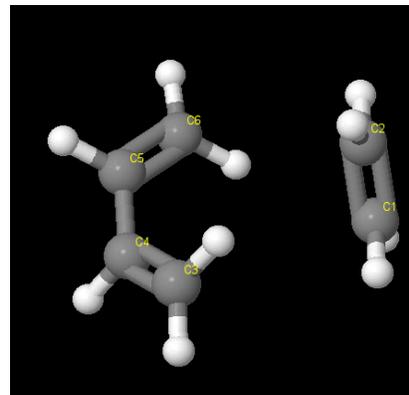


Image 1.31 (Substrate)



GIF 1.31

2. Stereochemistry: stereospecificity of the reaction

⁵ Gif 1.31 <https://drive.google.com/file/d/1UOHvS3E1J-uYyL2A6kWcgRT15UhgjxXG/view?usp=sharing>

The Diels Alder reaction is a stereospecific reaction in nature. The stereochemistry of the substrate will reflect in the stereochemistry of the product. It depends on the stereochemistry of both diene and dienophiles.

2.1 Stereochemistry of Dienophiles

The stereochemistry of the dienophile will appear in the product if the **dienophile is cis then the product will also be cis and same case with trans** isomer. This can be understood by the example of the reaction of **butadiene with dimethyl maleate and dimethyl fumarate**.

Here in the reaction of butadiene with dimethyl maleate the stereochemistry of the dienophile is cis so the product will also form with cis stereochemistry and same with the dimethyl fumarate the dienophile is trans so the product will also in trans form.

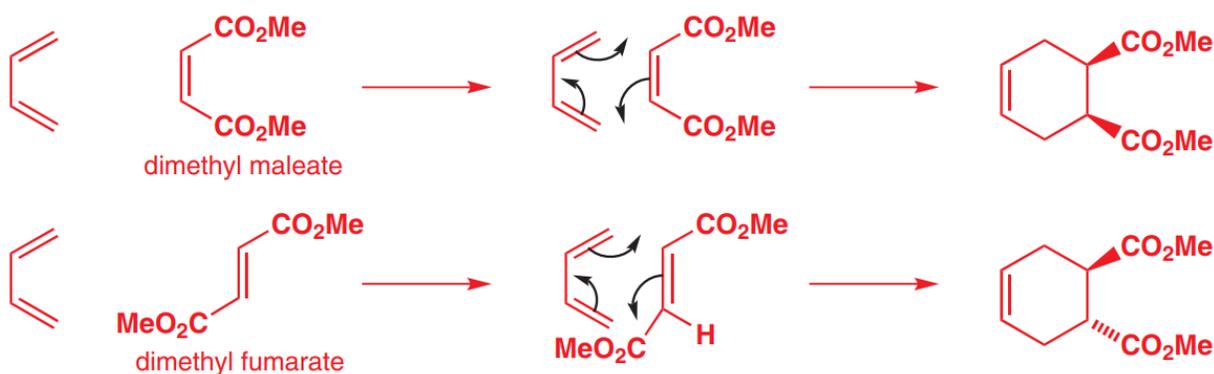
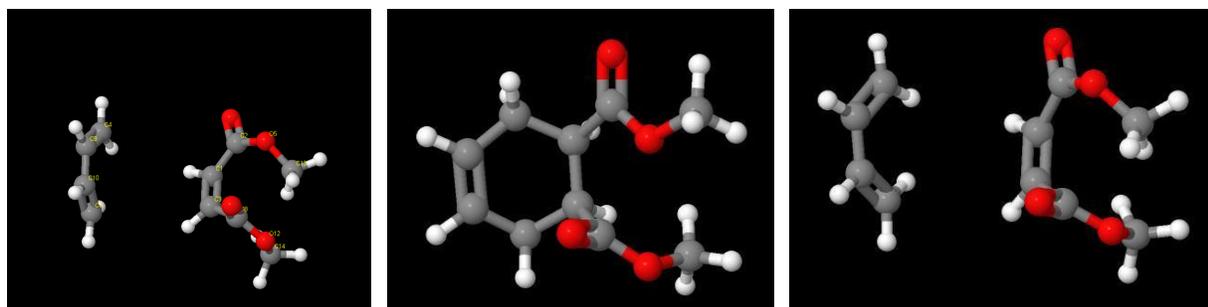


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

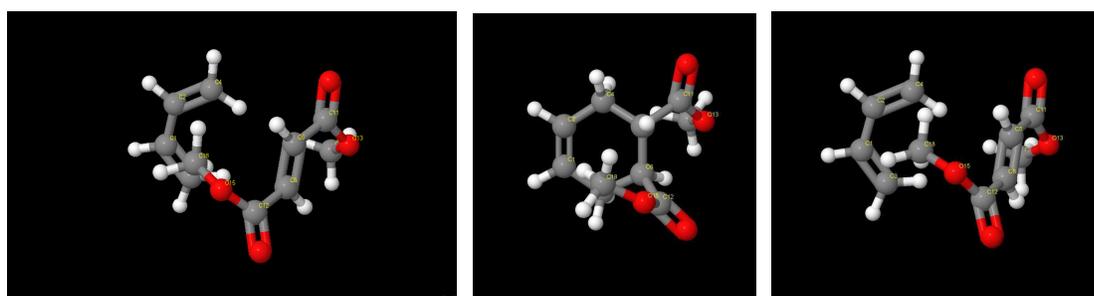
2.1



GIF 2.11

Image 2.11 (Product)

Image 2.12 (Substrate)



GIF 2.12

Image 2.13 (Product)

Image 2.14 (Substrate)

In the second example as per the bottom face approach the p-orbital of the diene will bind with the p-orbital of the dienophile from top side and form a new sigma bond so as H atom in the substrate is cis to the CO₂Me so it will remain cis in the product also so the product will be in the trans form as shown in the below given figure 2.12

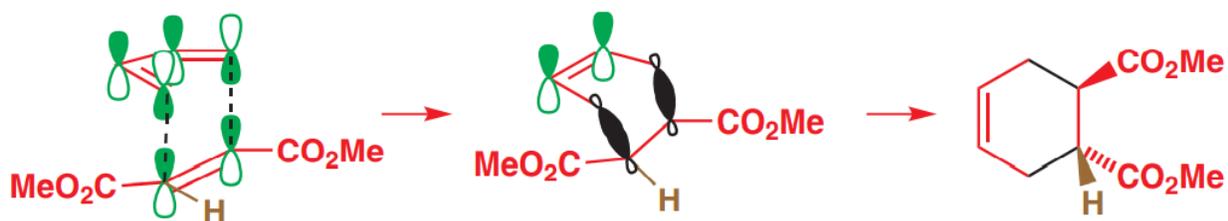


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

2.12

⁶ Gif 2.11 <https://drive.google.com/file/d/1qTxElS7TsOZ2gNisJKrXRE3HqF-VraIY/view?usp=sharing>

⁷ Gif 2.12 https://drive.google.com/file/d/1yhQuam73gaceFwSXLwqKqLXyu6Z_ghEy/view?usp=sharing

As shown in the figure the dienophile will remain as it is in the transition state also and the same will appear in the product.

2.2 Stereochemistry of the diene

There are three possibilities of Stereochemical arrangement in Dienes due to the presence of the two pi-bonds.

- 1) cis-cis
- 2) trans-trans
- 3) cis-trans

so for the explanation of the cis-cis diene stereochemistry we can take the example of the below given reaction.

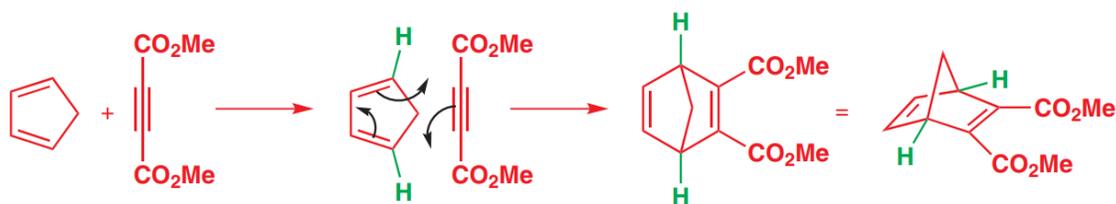
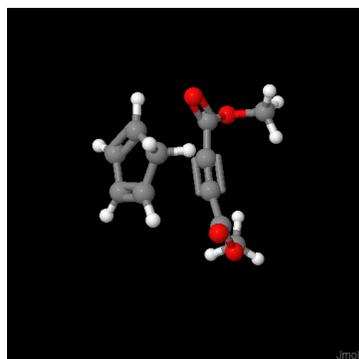


Image taken from "ORGANIC CHEMISTRY " by JONATHAN CLAYDEN,NICK GREEVES AND STUART WARREN

2.21



GIF 2.21

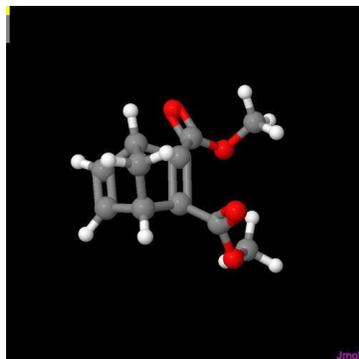


Image 2.21 (Product)

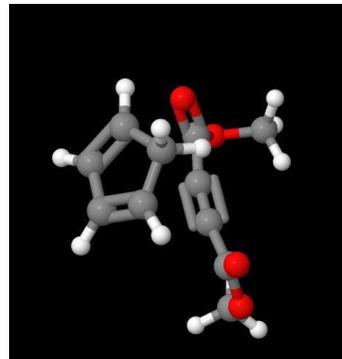


Image 2.22 (Substrate)

8

In the above given reaction there are two pi-bond in the pentadiene is in the cis form and the two hydrogens at the terminal of the pi-bonds will remain in the same position as it is in the substrate and here in the cis-cis form the symmetry of the substrate is preserved and appears same as it is in the product.

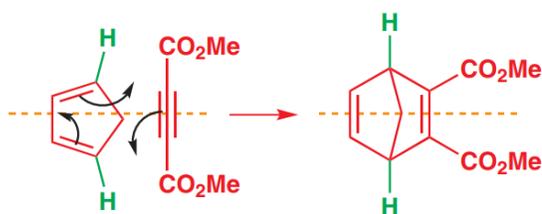


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

2.22

The trans-trans is also a symmetrical arrangement so in this also symmetry will be preserved, and the product will also be symmetrical. The below given reaction can be used to explain the stereochemistry of trans-trans diene.

⁸ Gif 2.21 <https://drive.google.com/file/d/1juhPzMo-CML0a5wYseLh0QM0z-0yLmTG/view?usp=sharing>

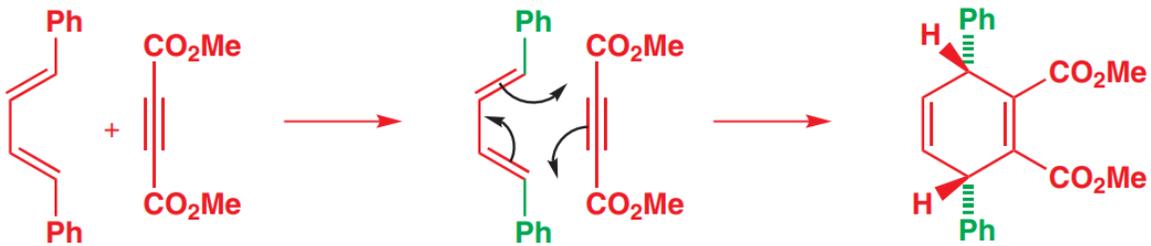
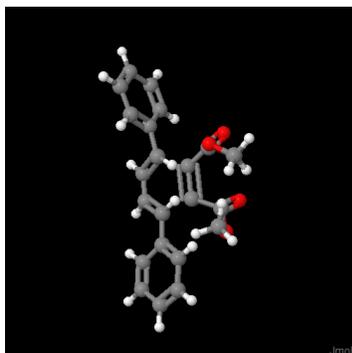


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

2.23



GIF 2.22

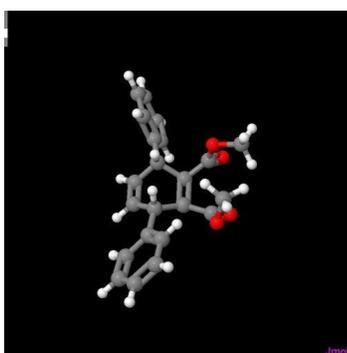


Image 2.23 (Product)

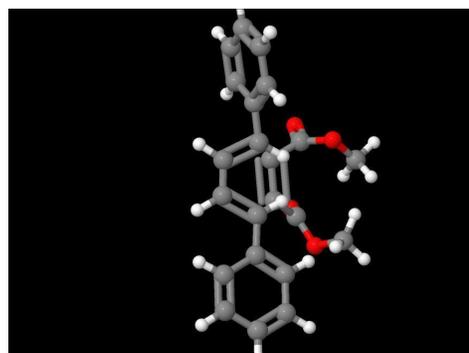
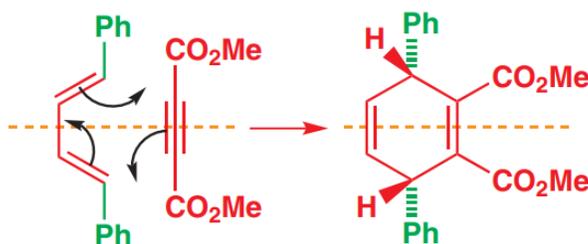


Image 2.24 (Substrate)

9

The trans-trans arrangement in the substrate will also appear in the product, phenyl group will be at the back side in the product so the trans-trans arrangement can be maintained and the product is also symmetrical.



2.24

⁹ Gif 2.22 <https://drive.google.com/file/d/1d81BsShoB3L1v-ST30vBKuCbqu26Vux/view?usp=sharing>

The **cis-trans** arrangement is the unsymmetrical so the product will also be the unsymmetrical and in the product also that cis-trans will be maintained from the below given reaction that can be understood.

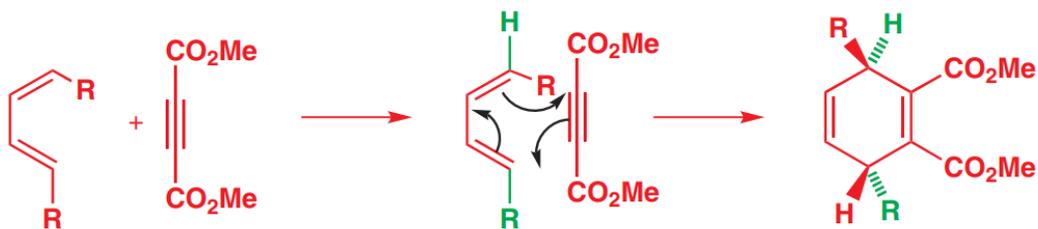
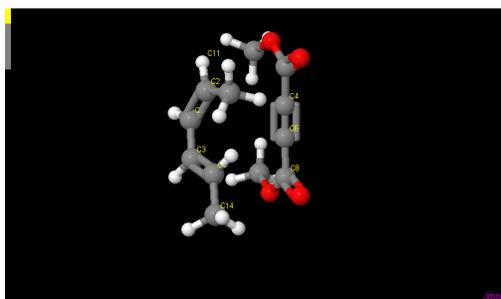


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2.25



GIF 2.23

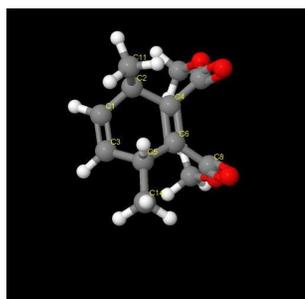


Image 2.25 (Product)

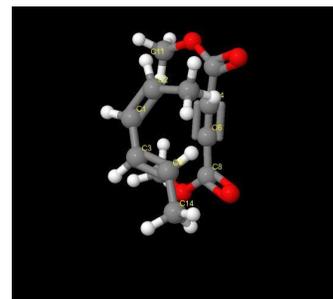


Image 2.26 (Substrate)

10

The dienophile will approach from bottom side so the R group will remain above and at the another end it will approach from above so the R group will remain bottom side so the cis-trans stereochemical arrangement will also be appeared in the product.

So, from the above **three cases** it can be concluded that stereochemical arrangement of the substrate will be preserved and appear in the product.

3. The Endo-rule for Diels Alder Reaction

¹⁰ Gif 2.23 <https://drive.google.com/file/d/1Mf92KKZ-Xd86SALCB58109vC6pVclslc/view?usp=sharing>

The endo rule can be understood easily by the reaction of maleic anhydride and cyclopentadiene. There are two possible products of the reaction i.e., endo and exo product but the endo product will only form.

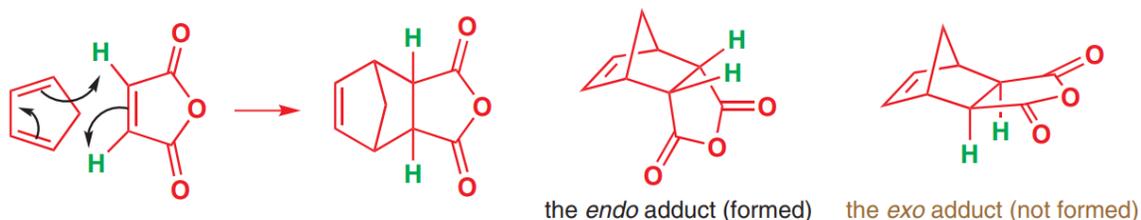
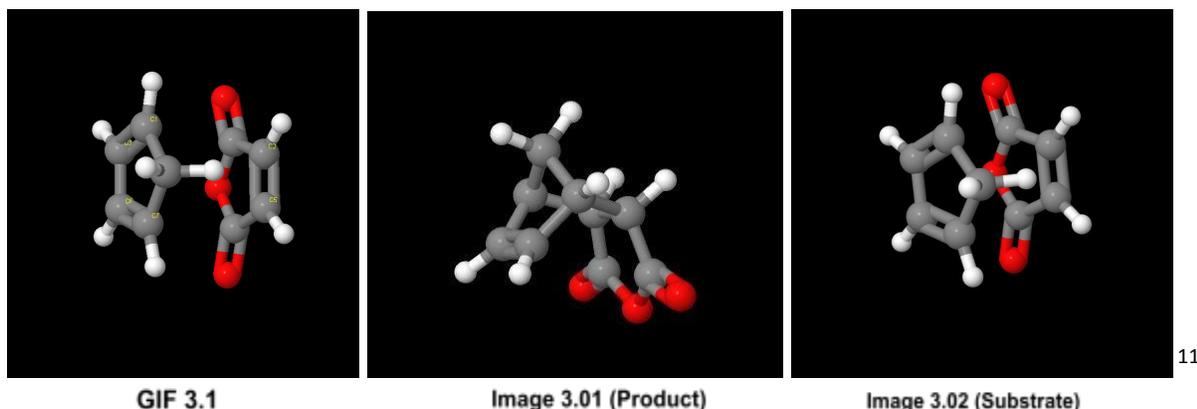


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

3.1



To understand the reason for forming the endo product we have to study about the formation of the endo and exo product. The endo and exo addition will be occurred as shown below in the figure 3.2, in the endo addition there will be a secondary orbital interaction of diene with the dienophile having activating substituent and in the exo addition there is no such secondary orbital interaction therefore the endo product is preferred over the exo product.

¹¹ Gif 3.1 <https://drive.google.com/file/d/1hkn1hIHQFBPmNcB8V7fPDyEhysybBBxA/view?usp=sharing>

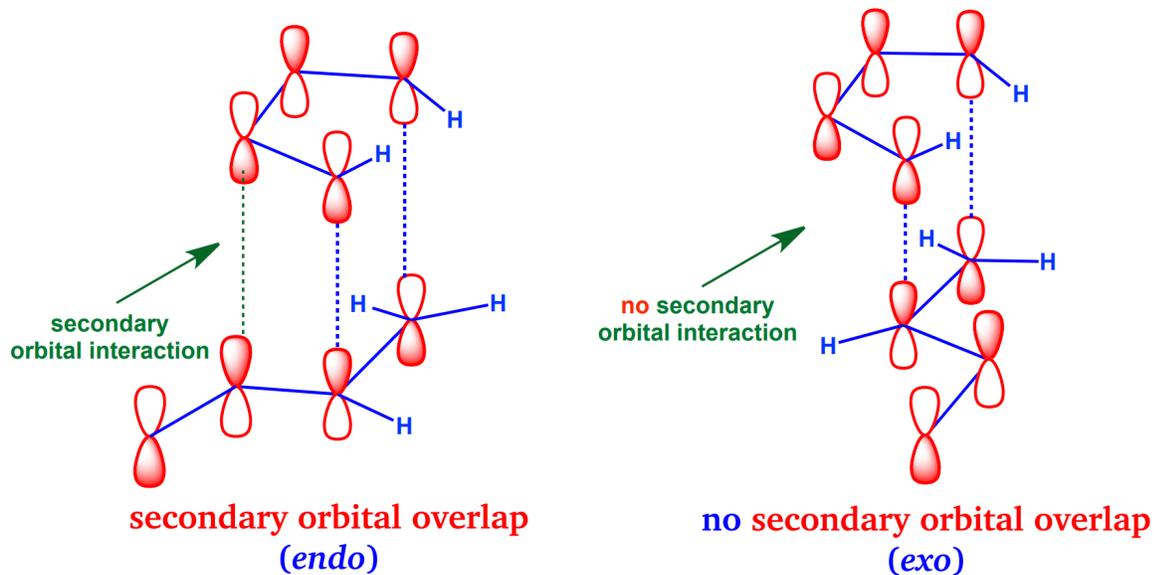
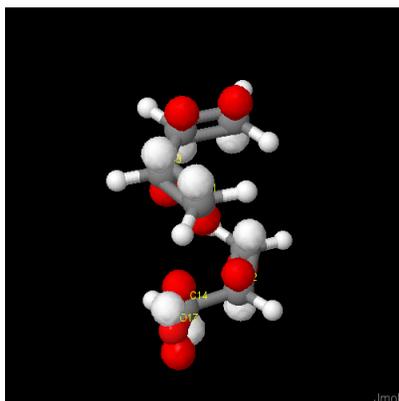


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3.2

Endo Addition:



GIF 3.2

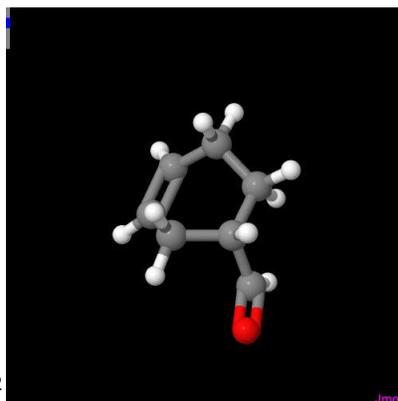


Image 3.03 (Product)

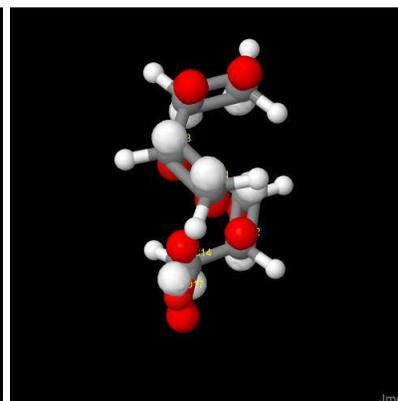
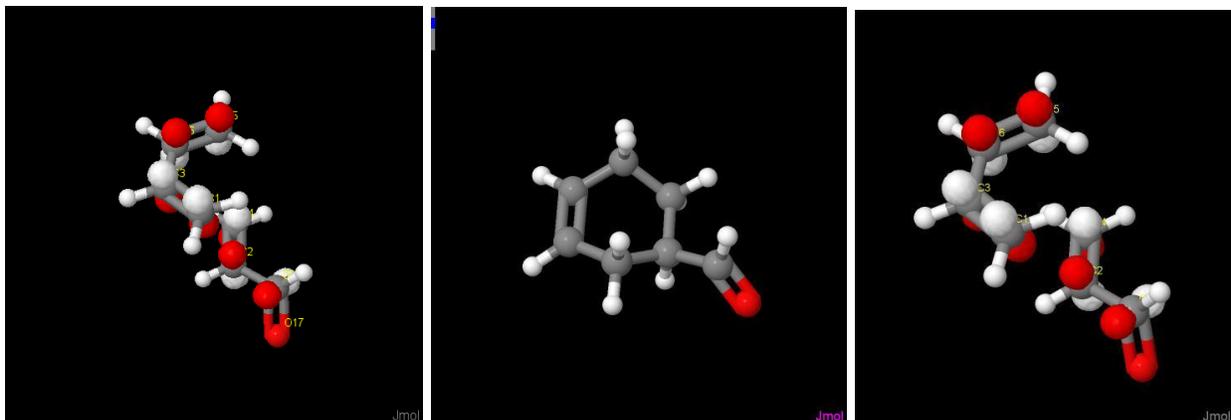


Image 3.04 (Substrate)

Exo Addition:

¹² Gif 3.2 https://drive.google.com/file/d/119Lwjwcl_klESXkktk6-DAduv3z0dAudD/view?usp=sharing



13

GIF 3.3

Image 3.05 (Product)

Image 3.06 (Substrate)

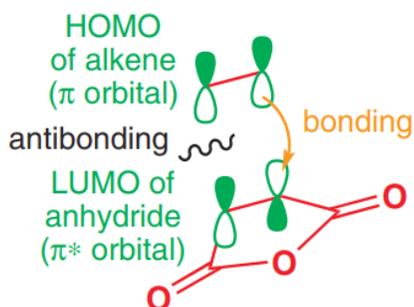
As there is more steric hindrance in the endo product than the exo product so the endo product is less stable than the exo product then also the endo product is forming due to it forming through the kinetic process. In the endo product there is a secondary orbital overlap which decreases the energy of the transition state, so the endo product is preferred over the exo product.

4. Frontier orbital description of cycloadditions

In the cycloaddition reaction two new sigma bonds will form in the product so there should be two filled and two empty orbitals in the substrate at the correct place and correct symmetry. So, we have to try different arrangements of HOMO and LUMO between diene and dienophile. There should be bonding arrangements at both the sites of bonding between orbitals. We have to take one as HOMO and another as LUMO.

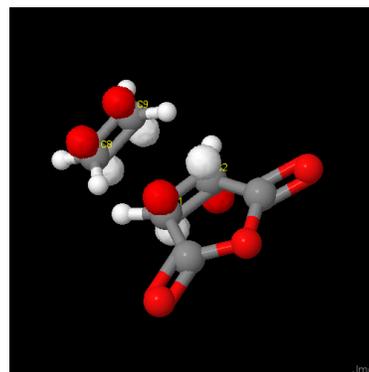
¹³ Gif 3.3 <https://drive.google.com/file/d/1AzUSJMx0QimEv-HFdbpUcoPMWL4Vonwi/view?usp=sharing>

Let us take the HOMO for the alkene and the LUMO for the dienophile of the below given reaction of the ethene and the maleic anhydride. As there is alkene here in place of diene there is one bonding and one antibonding arrangement is possible so this reaction will not proceed.



14 Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

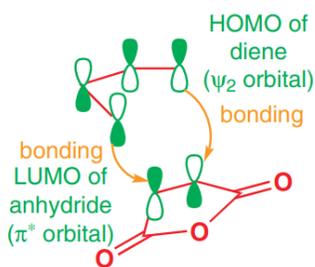
4.1



GIF 4.1

Now if we exchange the diene with alkene i.e. HOMO of the diene and LUMO of the dienophile then there will be two bonding interactions in between them. Now we can make different arrangement of the orbitals according to the symmetry for getting the good arrangement of both HOMO and LUMO so as shown in the below figure we can arrange the orbitals of diene with starting from zero nodes and increasing one by one and as per the below figure the first possible arrangement is good due to having lesser energy gap so there will be better overlap of orbitals.

Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN



4.2

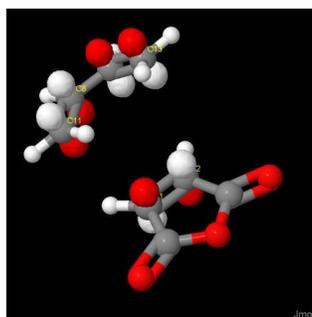


Image 4.01 (Substrate)

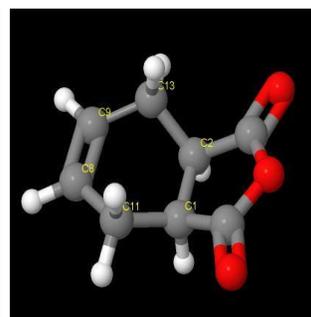
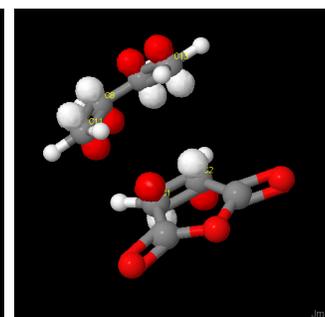


Image 4.02 (Product)



GIF 4.2

¹⁴ Gif 4.1 <https://drive.google.com/file/d/10aXyfiMKERIHbBhRM5AEq60G4CTbr8ml/view?usp=sharing>
Gif 4.2 https://drive.google.com/file/d/1lPMDB8c2HxJekf9Jhz_hZ7l3p4QGxgfD/view?usp=sharing

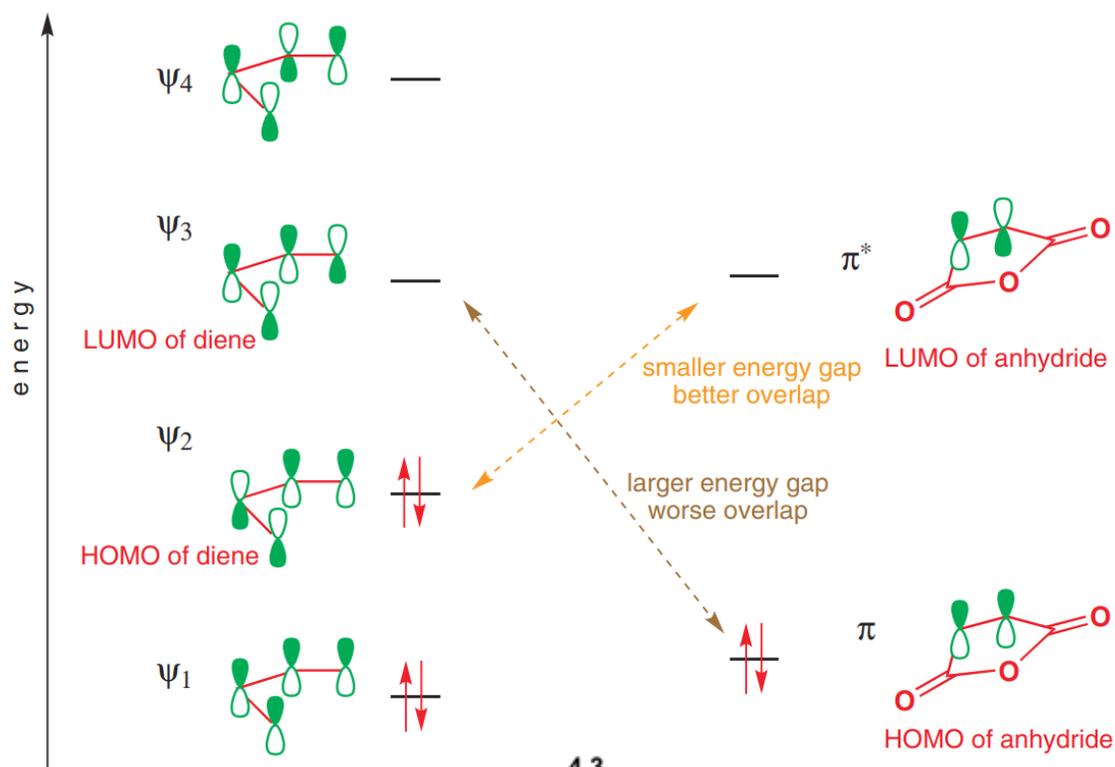


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

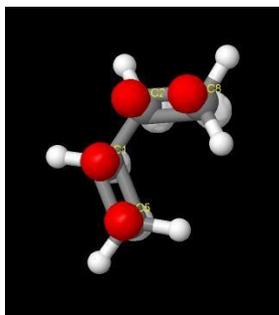


Image 4.03 (si-1)

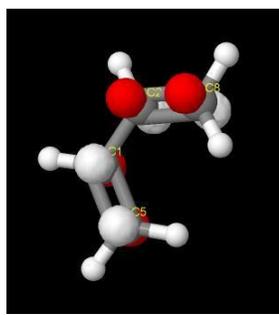


Image 4.04 (Si-2)
HOMO of Diene

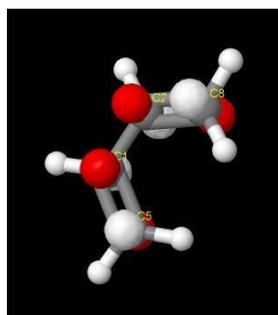


Image 4.05 (Si-2)
LUMO of Diene

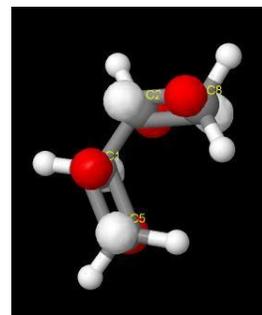


Image 4.06 (Si-4)

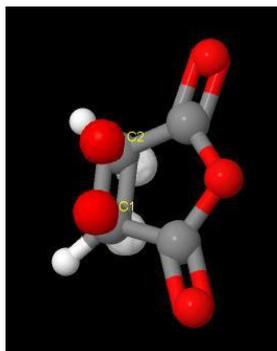


Image 4.07 (pi)
HOMO of anhydride

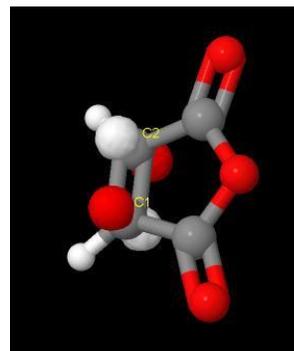


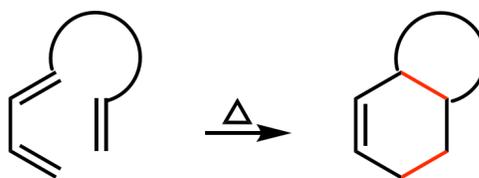
Image 4.08 (pi-star)
LUMO of anhydride

5. Intramolecular Diels–Alder reactions

In Intramolecular type of reaction when the diene and dienophiles are in the same molecule then there is no more difficulty in pursuing a Diels alder reaction. In this type of reaction endo rule will not be followed so exo product will be preferred because there is no conjugation group on the dienophile so there would be absence of orbitals which can bind with the back of the diene.

There are two types of intramolecular Diels alder reaction.

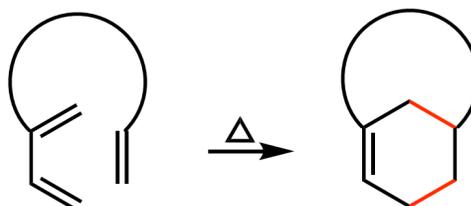
1) **Type I IMDA:** In this type there is formation of fused bicyclic ring by connection of dienophile with C1 of the diene as shown in the below given fig.



Fused bicyclic system

5.1 Image taken from slides provided by Prof. Krishna P Kaliappan

2) **Type II IMDA:** In this type there is formation of bridged bicyclic ring by connection of dienophile with C2 of the diene and the ring formed should be greater than the six membered ring (minimum 7 membered ring) as shown in the below given fig.



Bridged bicyclic system

5.2 Image taken from slides provided by Prof. Krishna P Kaliappan

IMDA Type 1 examples:

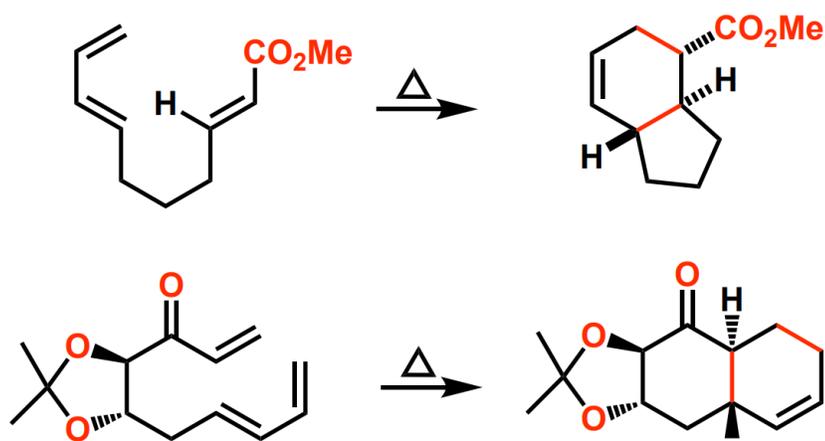
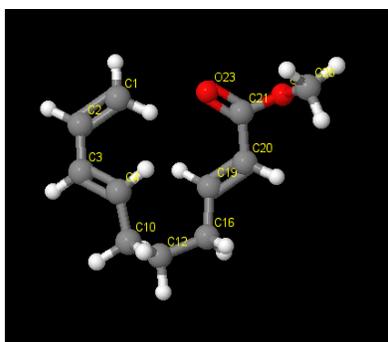


Image taken from slides provided by Prof. Krishna P Kaliappan
5.3

¹⁵Reaction 1:



GIF 5.1

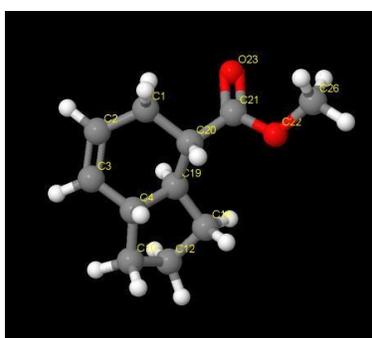


Image 5.02 (Product)

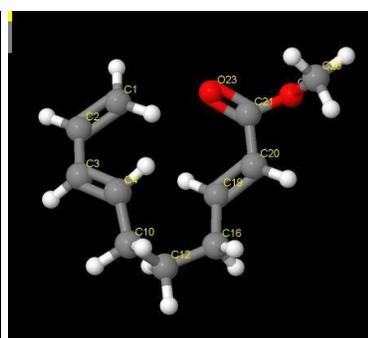
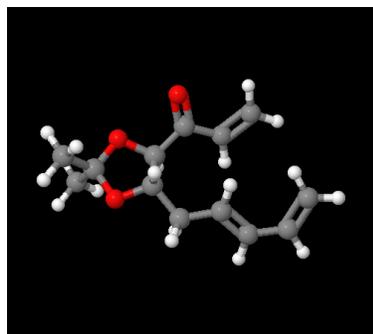


Image 5.01 (Substrate)

¹⁶Reaction 2:



GIF 5.2

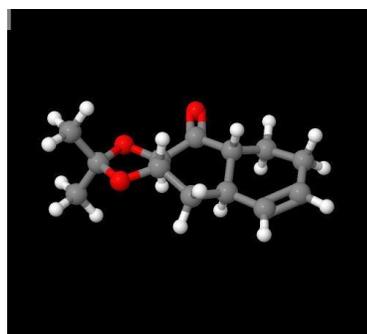


Image 5.04 (Product)

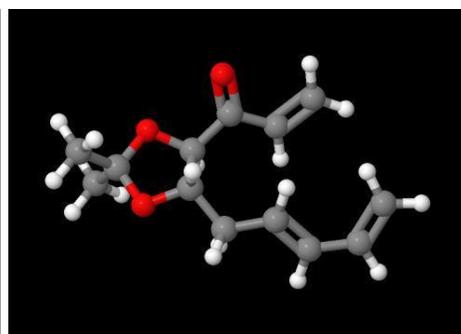


Image 5.03 (Substrate)

¹⁵ Gif 5.1 https://drive.google.com/file/d/11DkAuWijt_Al51BUocpi6Sxc0Ym5n1au/view?usp=sharing

¹⁶ Gif 5.2 <https://drive.google.com/file/d/1vMzIHp9pEeiWoe1QpXNb4xDfNwyfEaqK/view?usp=sharing>

IMDA Type 2 examples:

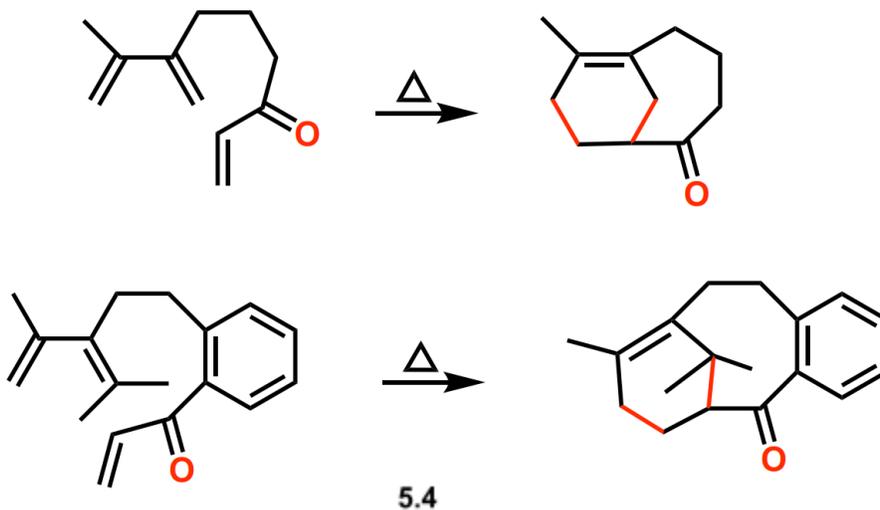
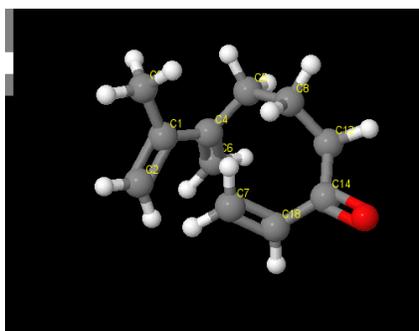


Image taken from Slides provided by Prof. Krishna P. Kaliappan

¹⁷Reaction 1:



GIF 5.3

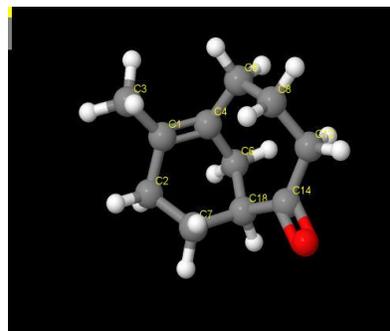


Image 5.03 (Product)

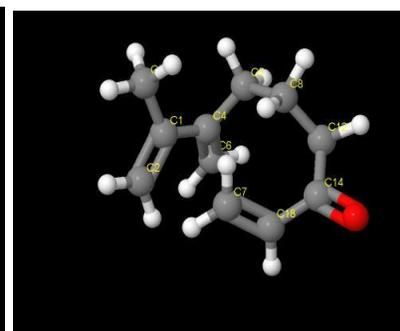
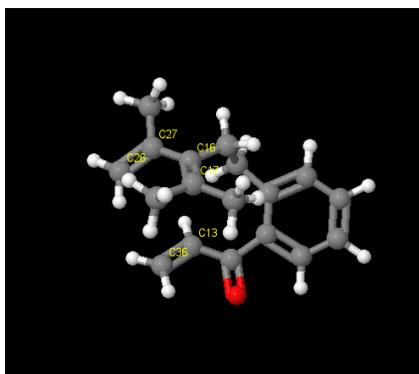


Image 5.04 (Substrate)

¹⁸Reaction 2:



GIF 5.4

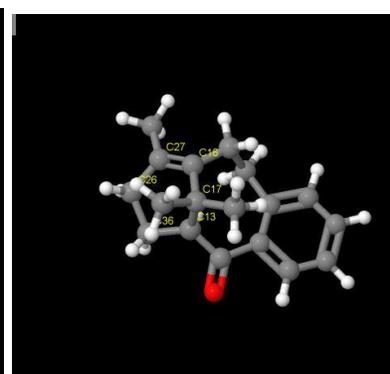


Image 5.06 (Product)

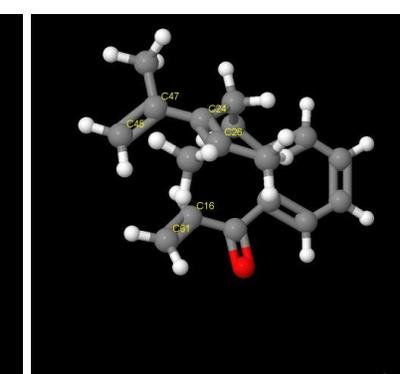


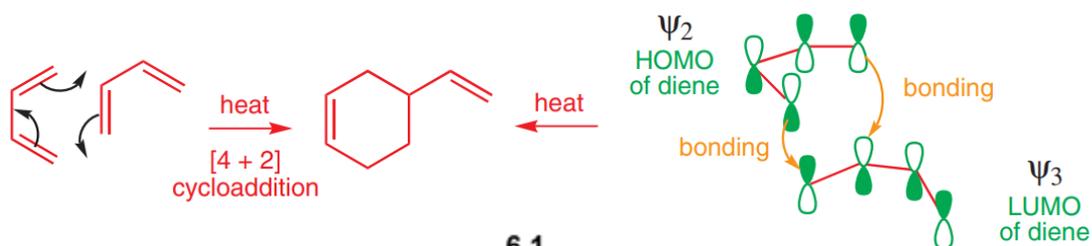
Image 5.05 (Substrate)

¹⁷ Gif 5.3 <https://drive.google.com/file/d/1eRbuRxmWfQSyUGo800mYPhzKf8PR30IC/view?usp=sharing>

¹⁸ Gif 5.4 <https://drive.google.com/file/d/18TzVyIHcfjEoh0u7CKDUJOCvIcKfTSOM/view?usp=sharing>

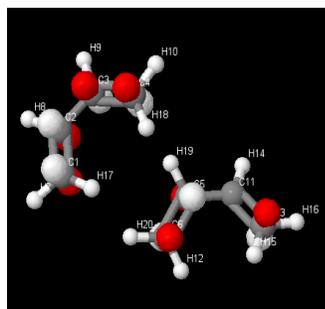
6. Dimerization of dienes by cycloaddition reactions

The dienes can react with each other as they have high energy HOMO and low energy LUMO so one of the dienes will act as diene and double bond of another diene will act as a dienophile and the [4+2] cycloaddition will result into the cyclic structure as shown in the below given figure.



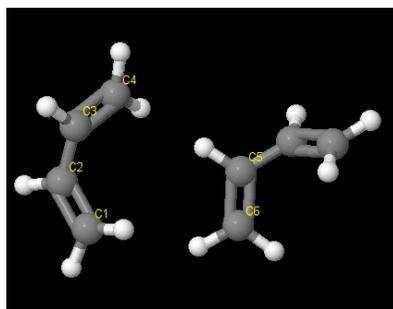
6.1

Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN



1920

GIF 6.1



GIF 6.2

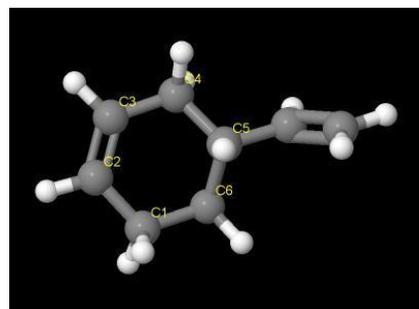


Image 6.01 (Product)

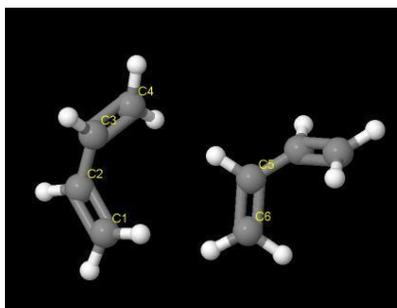


Image 6.02 (Substrate)

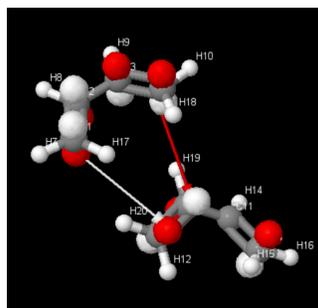


Image 6.03

¹⁹ Gif 6.1 <https://drive.google.com/file/d/166flkCPGXSl7Aca7oRkrOsER0o8AgiAi/view?usp=sharing>

²⁰ Gif 6.2 <https://drive.google.com/file/d/15jNyDHAL-X2A4bR5pZMR5TXeHSiY2Xu0/view?usp=sharing>

7. Regioselectivity in Diels–Alder reactions

In the Diels-Alder reaction the dienophile will have the electron withdrawing group so at the next end of the double electron deficient center will be generated and similarly in the diene whichever double bond contains the electron donating group end of the that double contains the electron rich center so the electron rich center and electron deficient center will form a bond.

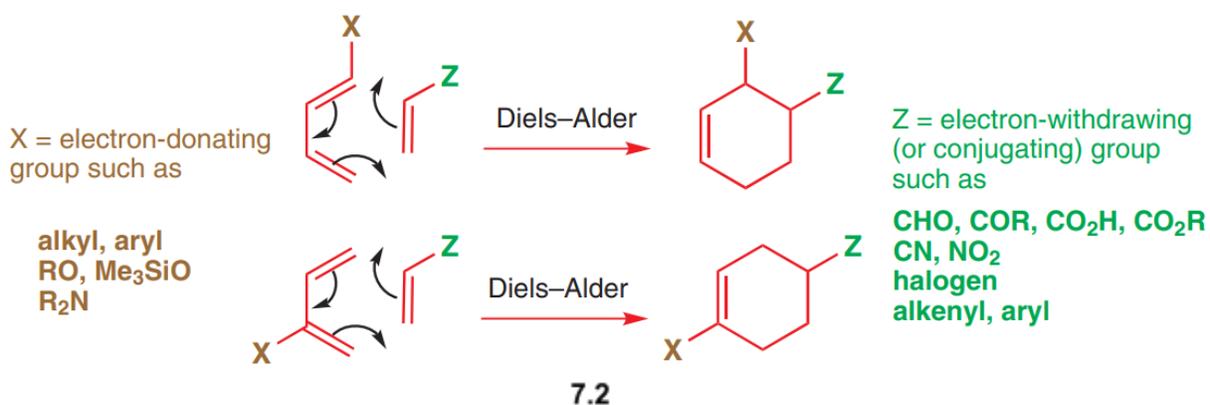
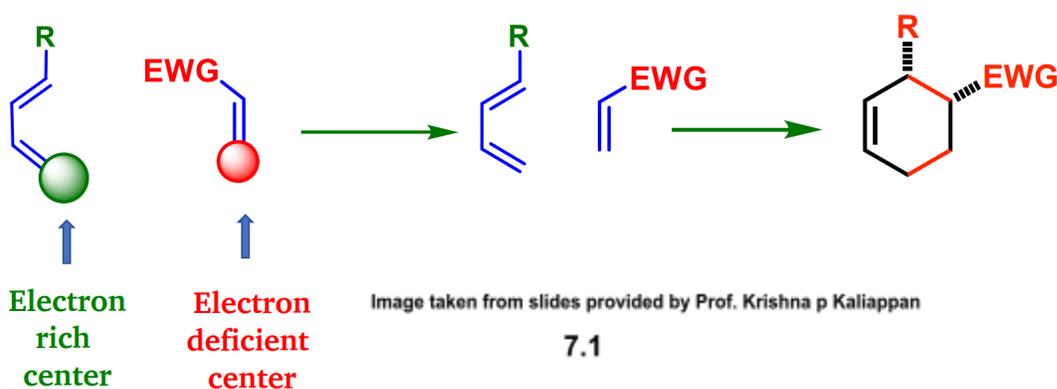


Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN

So as shown in the above figure the Diels-Alder reaction will proceed in the regioselective manner which can be explained by some examples.

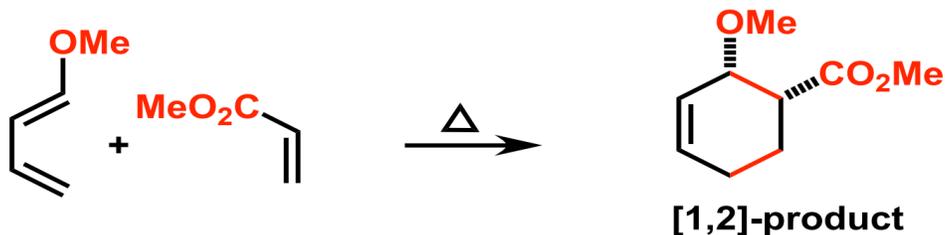
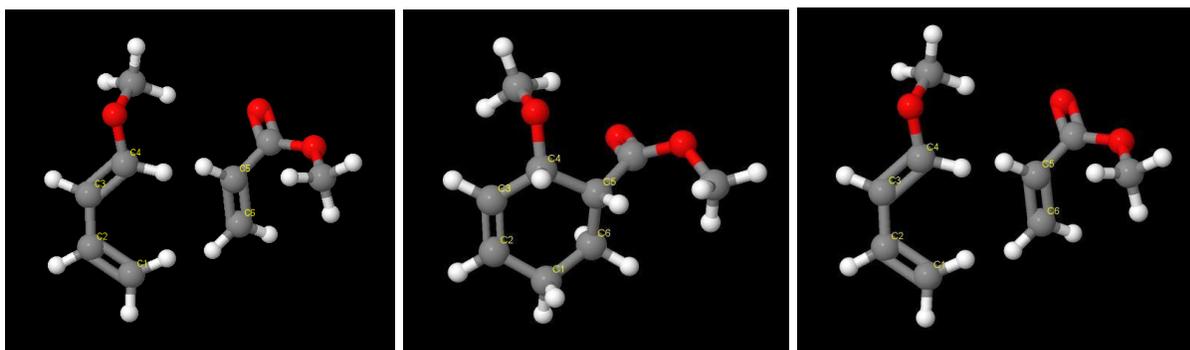


Image taken from Slides provided by Prof. Krishna P Kaliappan

7.3



GIF 7.0

Image 7.01 (Product)

Image 7.02 (Substrate)

21

8. The Woodward–Hoffmann description of the Diels–Alder reaction

The Woodward-Hoffmann rule is “**In a thermal pericyclic reaction the total number of (4q + 2)s and (4r)a components must be odd**” and let us try to understand some terminology first.

The (4q+2) and (4r) refers to the number of electrons in the component in which the q and r are the integers. In the above formula the “s” and “a” refers to the suprafacial and antarafacial respectively.

Suprafacial: The condition in which the orbital overlaps with each other by the same

²¹ Gif 7.0 <https://drive.google.com/file/d/1WA9V2urIU0V4pM-IqncfumQkZDFIftoE/view?usp=sharing>

face at both the ends.

Antarafacial: The condition in which the orbital overlaps with each other by the opposite face at both the ends.

Another way to explain the Woodward Hoffmann rule:

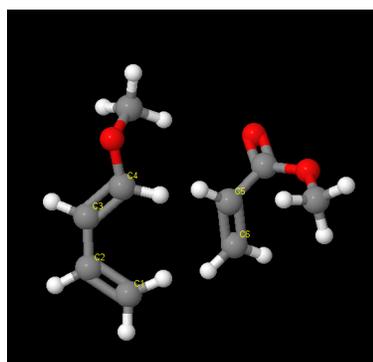
In the allowed thermal pericyclic reaction the sum of the number of suprafacial components and the number of antarafacial components must be odd.

Now let us apply the Woodward Hoffmann rule to the Diels alder reaction, for that we have to draw the orbitals of the both the ends of the diene and dienophile and have to draw the lines to join both the component and have to observe that whether it is suprafacial (s) or antarafacial (s) depending on the same or opposite side overlapping of the orbitals. Now let us put the values in the $(4q+2)s$ and $(4r)a$ No. of $(4q+2)s = 1$ and No. of $(4r)a = 0$ thus $0+1=1$ (odd) thus the Diels alder reaction is allowed thermally.



8.1

Image taken from "ORGANIC CHEMISTRY" by JONATHAN CLAYDEN, NICK GREEVES AND STUART WARREN



GIF 8.0

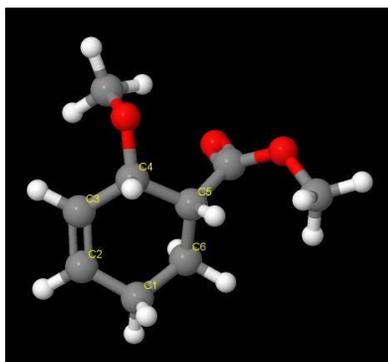


Image 8.01 (Product)

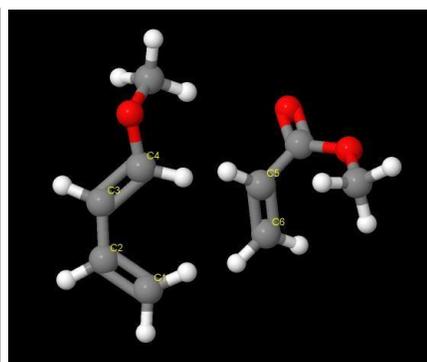


Image 8.02 (Substrate)

22

²² Gif 8.0 https://drive.google.com/file/d/1_0ox6qZ6L_Owg1uG30_vDqjODrH_dCBQ/view?usp=sharing

Conclusion:

The Diels-Alder reaction is stereospecific with respect to substituent configuration in both the dienophile and the diene. In some Diels-Alder reactions regioselectivity is seen. It is necessary to understand the stereochemistry of the reaction in the 3D form. Open source 3D visualization software such as Jmol can be very helpful in understanding this concept. The endo and exo product formation in a reaction involving bicyclic product can also be clearly identified by modeling in Jmol. From the above work it can be concluded that Jmol is a very useful tool for understanding the stereochemistry of Diels-Alder reactions.

Scripts:

1. Gif 1.11

```
capture "D:\Tahirali\FOSSE-SOUL\Diels alder\Jmol files\animation1.gif" loop ; move 0 10 0 0 0 0 0 10;
delay 4; connect @2 @4 single;connect @7 @5 single; connect @2 @4 partial 2.2 radius 0.1; connect
@7 @5 partial 2.2 radius 0.1; connect @3 @1 partial 2.2 radius 0.1;minimize; delay 4; connect @1 @2
single; connect @3 @7 single; connect @1 @3 double; connect @7 @5 single;connect @2 @4 single;
connect @4 @5 single;move 0 -10 0 0 0 0 0 10;
```

2. Gif 1.12

```
Capture "D:\Tahirali\FOSSE-SOUL\Diels alder\Jmol files\General Description\Maleic anhydride &
butadiene" loop 60;move 0 10 0 0 0 0 0 10; minimize;delay 2; connect @2 @7 single; connect @4 @5
single; connect @4 @5 partial 2.2 radius 0.1; connect @2 @7 partial 2.2 radius 0.1; connect @1 @3
partial 2.2 radius 0.1;minimize;delay 4;move 0 -10 0 0 0 0 0 10; connect @1 @3 double; connect @ 1
@2 single; connect @3 @4 single; connect @4 @5 single; connect @7 @5 single; connect @2 @7
single;delay 4
```

3. Gif 1.21

```
capture "D:\Tahirali\FOSSE-SOUL\Diels alder\Jmol files\Dienes and Dienophiles\Dienes\animation
S-T-P.gif" loop 60;move 0 10 0 0 0 0 0 10; minimize;delay 2; connect @3 @1 single; connect @6 @2
```

single; connect @3 @1 partial 2.2 radius 0.1; connect @6 @2 partial 2.2 radius 0.1; connect @4 @5 partial 2.2 radius 0.1; minimize; delay 4; move 0 -10 0 0 0 0 0 10; connect @4 @5 double; connect @4 @3 single; connect @1 @3 single; connect @1 @2 single; connect @2 @6 single; connect @6 @5 single; delay 4

4. Gif 1.22

select @3; select @1; rotate branch {C3} {C1} 180 30;

5. Gif 1.31

capture "D:\Tahirali\FOSSE-SOUL\Diels alder\Jmol files\Dienes and Dienophiles\Dienophiles\animation S-T-P.gif" loop 60; move 0 10 0 0 0 0 0 10; minimize; delay 2; connect @3 @1 single; connect @6 @2 single; connect @3 @1 partial 2.2 radius 0.1; connect @6 @2 partial 2.2 radius 0.1; connect @4 @5 partial 2.2 radius 0.1; minimize; delay 4; move 0 -10 0 0 0 0 0 10; connect @4 @5 double; connect @4 @3 single; connect @1 @3 single; connect @1 @2 single; connect @2 @6 single; connect @6 @5 single; delay 4

6. Gif 2.11

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Butadiene+d.maleate\anim.gif" loop 60; delay 2; connect @4 @1 single; connect @7 @3 single; connect @4 @1 partial 2.2 radius 0.1; connect @7 @3 partial 2.2 radius 0.1; connect @9 @10 partial 2.2 radius 0.1; minimize; delay 4; connect @4 @1 single radius 0.15; connect @7 @3 single radius 0.15; connect @1 @3 single; connect @10 @7 single; connect @9 @4 single; connect @10 @9 double; minimize

7. Gif 2.12

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Butadiene + d.fumarate\anim.gif" loop 60; delay 2; connect @4 @5 single; connect @3 @6 single; connect @4 @5 partial 2.2 radius 0.1; connect @3 @6 partial 2.2 radius 0.1; connect @1 @2 partial 2.2 radius 0.1; minimize; delay 4; connect @4 @5 single radius 0.15; connect @3 @6 single radius 0.15; connect @1 @3 single; connect @2 @4 single; connect @6 @5 single; connect @1 @2 double; minimize

8. Gif 2.21

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Dienes\cis-cis\anim.gif" loop 60; delay 2; connect @2 @1 single; connect @6 @3 single; connect @2 @1 partial 2.2 radius 0.1; connect @6 @3 partial 2.2 radius 0.1; connect @5 @7 partial 2.2 radius 0.1; minimize; connect @2

@1 single radius 0.15;connect @6 @3 single radius 0.15;connect @5 @2 single;connect @5 @7 double;connect @7 @6 single;connect @1 @3 double;minimize

9. Gif 2.22

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\anim.gif" loop 60;delay 2;Connect @4 @5 single; connect @1 @6 single;connect @4 @5 partial 2.2 radius 0.1;connect @1 @6 partial 2.2 radius 0.1;connect @2 @3 partial 2.2 radius 0.1;minimize;delay 2;connect @4 @5 single radius 0.15;connect @1 @6 single radius 0.15;connect @3 @4 single;connect @3 @2 double;connect @2 @1 single;connect @6 @5 double;minimize;

10. Gif 2.23

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Dienes\cis-trans\anim.gif" loop 60;delay 2;Connect @2 @4 single; connect @5 @6 single;connect @2 @4 partial 2.2 radius 0.1;connect @5 @6 partial 2.2 radius 0.1;connect @1 @3 partial 2.2 radius 0.1;minimize;delay 2;connect @2 @4 single radius 0.15;connect @5 @6 single radius 0.15;connect @1 @2 single;connect @1 @3 double;connect @3 @5 single;connect @4 @6 double;minimize

11. Gif 3.1

Capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Dienes\cis-cis\anim.gif" loop 60;delay 2;Connect @1 @2 single; connect @5 @7 single;connect @1 @2 partial 2.2 radius 0.1;connect @5 @7 partial 2.2 radius 0.1;connect @3 @6 partial 2.2 radius 0.1;minimize;connect @1 @2 single radius 0.15;connect @5 @7 single radius 0.15;connect @3 @1 single;connect @3 @6 double;connect @6 @7 single;connect @2 @5 single;minimize

12. Gif 3.2

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Endo rule\anim.gif" loop 60;move 30 0 0 0 0 0 0 3;connect @5 @4 single;connect @5 @4 partial 1.1 radius 0.05; connect @1 @2 single;connect @1 @2 partial 1.1 radius 0.05;connect @3 @14 single;connect @3 @14 partial 1.1 radius 0.05;move -30 0 0 0 0 0 0 3;delay 2;move 0 20 0 0 0 0 0 5;connect @3 @14 delete;connect @5 @4 single radius 0.15;connect @1 @2 single radius 0.15;select @5;lcaocartoon delete;select @6;lcaocartoon delete;select @3;lcaocartoon delete;select @1;lcaocartoon delete;select @4;lcaocartoon delete;select @2;lcaocartoon delete;select @14;lcaocartoon delete;select @17;lcaocartoon delete;connect @6 @5 single radius

0.15;connect @3 @1 single radius 0.15;connect @4 @2 single radius 0.15;connect @6 @3 double;minimize;

Orbitals

select @2;lcaocartoon color white red create pz;
select @14;lcaocartoon color white red create pz;
select @5;lcaocartoon color white red create pz;
select @6;lcaocartoon color white red create pz;
select @3;lcaocartoon color red white create pz;
select @1;lcaocartoon color red white create pz;
select @4;lcaocartoon color red white create pz;
select @17;lcaocartoon color red white create pz;

13. Gif 3.3

Capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Endo rule\Exo addition\anim.gif"
loop 60;move 30 0 0 0 0 0 0 0 3;connect @1 @2 single;connect @5 @4single;connect @1 @2 partial 1.1 radius 0.05;connect @5 @4 partial 1.1 radius 0.05;move -30 0 0 0 0 0 0 0 3;delay 2;move 0 20 0 0 0 0 0 0 5;connect @1 @2 single radius 0.15;connect @5 @4 single radius 0.15;delay 2;select @5;lcaocartoon delete;select @6;lcaocartoon delete;select @3;lcaocartoon delete;select @1;lcaocartoon delete;select @4;lcaocartoon delete;select @2;lcaocartoon delete;select @9;lcaocartoon delete;connect @6 @5 single radius 0.15;connect @3 @1 single radius 0.15;connect @4 @2 single radius 0.15;connect @6 @3 double;minimize

Orbitals

select @4;lcaocartoon color red white create pz;
select @1;lcaocartoon color red white create pz;
select @3;lcaocartoon color red white create pz;
select @5;lcaocartoon color white red create pz;
select @6;lcaocartoon color white red create pz;

```
select @2;lcaocartoon color white red create pz;  
select @9;lcaocartoon color white red create pz;
```

13. Gif 4.1

```
capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Dienes\cis-trans\anim.gif"  
loop 90;delay 3;draw arrow1 arrow {-0.718 1.9 -2.99} {1.0 1.3 0.3}radius 0.06 color red
```

14. Gif 4.2

```
capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Dienes\cis-trans\anim.gif"  
loop 90;delay 3;draw arrow1 arrow {-2.244 2.370 -0.531} {0.5 1.25 -0.283}radius 0.06 color red; draw  
arrow2 arrow {-2.212 -0.658 -0.248} {0.7 -0.194 0.241} radius 0.06 color white;delay 4;draw arrow1  
delete;draw arrow2 delete;select @13;lcaocartoon delete;select @9;lcaocartoon delete;select  
@8;lcaocartoon delete;select @11;lcaocartoon delete;select @2;lcaocartoon delete;select  
@1;lcaocartoon delete;Connect @2 @13 single; connect @11 @1 single;connect @2 @13 partial 2.2  
radius 0.1;connect @11 @1 partial 2.2 radius 0.1;connect @9 @13 partial 2.2 radius 0.1;minimize;delay  
2;connect @2 @13 single radius 0.15;connect @1 @11 single radius 0.15;connect @11 @8  
single;connect @9 @13 single;connect @1 @2 single;connect @9 @8 double;minimize
```

15. Gif 5.1

```
Capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\IMDA\IMDA Type 1\anim.gif" loop  
60;delay 2;connect @1 @20 single;connect @1 @20 partial 2.2 radius 0.1;connect @4 @19  
single;connect @4 @19 partial 2.2 radius 0.1;connect @2 @3 partial 2.2 radius  
0.1;minimize;delay 2;connect @2 @3 double;connect @2 @1 single;connect @3 @4  
single;connect @1 @20 single radius 0.15;connect @4 @19 single radius 0.15;connect @19  
@20 single;minimize;
```

16. Gif 5.2

```
Capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\IMDA\IMDA Type 1\anim.gif" loop  
60;delay 2;connect @1 @2 single;connect @1 @2 partial 2.2 radius 0.1;connect @4 @6  
single;connect @4 @6 partial 2.2 radius 0.1;connect @5 @3 partial 2.2 radius  
0.1;minimize;delay 2;connect @5 @3 double;connect @2 @1 single radius 0.15;connect @6
```

@4 single radius 0.15;connect @6 @5 single radius 0.15;connect @3 @1 single radius 0.15;connect @4 @2 single;minimize;

17. Gif 5.3

Capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\IMDA\IMDA Type 1\anim.gif" loop 60;delay 2;connect @7 @2 single;connect @7 @2 partial 2.2 radius 0.1;connect @18 @6 single;connect @18 @6 partial 2.2 radius 0.1;connect @1 @4 partial 2.2 radius 0.1;minimize;delay 2;connect @1 @4 double;connect @2 @1 single radius 0.15;connect @6 @4 single radius 0.15;connect @6 @18 single radius 0.15;connect @7 @18 single radius 0.15;connect @7 @2 single radius 0.15;minimize;

18. Gif 5.4

Capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\IMDA\IMDA Type 1\anim.gif" loop 60;delay 2;connect @17 @13 single;connect @17 @13 partial 2.2 radius 0.1;connect @26 @36 single;connect @26 @36 partial 2.2 radius 0.1;connect @16 @27 partial 2.2 radius 0.1;minimize;delay 4;connect @16 @27 double;connect @26 @36 single radius 0.15;connect @17 @13 single radius 0.15;connect @26 @27 single radius 0.15;connect @13 @36 single radius 0.15;connect @17 @16 single radius 0.15;minimize;

19. Gif 6.1

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Stereospecificity\Dienes\cis-trans\anim.gif" loop 60;delay 2;Connect @5 @4 single; connect @1 @6 single;connect @5 @4 partial 2.2 radius 0.1;connect @1 @6 partial 2.2 radius 0.1;connect @2 @3 partial 2.2 radius 0.1;minimize;delay 2;connect @5 @4 single radius 0.15;connect @1 @6 single radius 0.15;connect @1 @2 single;connect @4 @3 single;connect @6 @5 single;connect @2 @3 double;minimize

20. Gif 6.2

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Dimerisation of diene\anim.gif" loop 60;move 30 0 0 0 0 0 0 0 3;draw arrow1 arrow {-0.641 1.589 0.475} {2.291 0.117 0.060} radius 0.05 color red;draw arrow2 arrow {-1.429 -1.251 -0.24} {2.212 -1.216 0.32} radius 0.06 color white;move 0 20 0 0 0 0 0 0 3;move -50 0 0 0 0 0 0 0 3;move 0 -30 0 0 0 0 0 0 3;select @4;lcaocartoon delete;select @3;lcaocartoon delete;select @2;lcaocartoon delete;select

@1;lcaocartoon delete;select @11;lcaocartoon delete;select @13;lcaocartoon delete;select @5;lcaocartoon delete;select @6;lcaocartoon delete;draw arrow1 arrow delete;draw arrow2 arrow delete;delay 2;Connect @5 @4 single; connect @1 @6 single;connect @5 @4 partial 2.2 radius 0.1;connect @1 @6 partial 2.2 radius 0.1;connect @2 @3 partial 2.2 radius 0.1;minimize;delay 2;connect @5 @4 single radius 0.15;connect @1 @6 single radius 0.15;connect @1 @2 single;connect @4 @3 single;connect @6 @5 single;connect @2 @3 double;minimize

21. Gif 7.0

capture "D:\FOSSEE SOUL IIT-BOMBAY\Diels alder\Jmol files\Frontier orbital descriptor\anim.gif" loop 60;delay 2;connect @4 @5 single; connect @1 @6 single; connect @4 @5 partial 2.2 radius 0.1; connect @1 @6 partial 2.2 radius 0.1; connect @3 @2 partial 2.2 radius 0.1;minimize;delay 4;connect @4 @5 single radius 0.15; connect @1 @6 single radius 0.15; connect @4 @3 single; connect @1 @2 single; connect @6 @5 single; connect @3 @2 double;minimize

22. Gif 8.0

capture "D:\Tahirali\FOSSEE-SOUL\Diels alder\Jmol files\Dienes and Dienophiles\Dienes\animation S-T-P.gif" loop 60;move 0 10 0 0 0 0 0 10; minimize;delay 2; connect @3 @1 single; connect @6 @2 single; connect @3 @1 partial 2.2 radius 0.1; connect @6 @2 partial 2.2 radius 0.1; connect @4 @5 partial 2.2 radius 0.1;minimize;delay 4;move 0 -10 0 0 0 0 0 10; connect @4 @5 double; connect @4 @3 single; connect @1 @3 single; connect @1 @2 single; connect @2 @6 single; connect @6 @5 single;delay 4

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