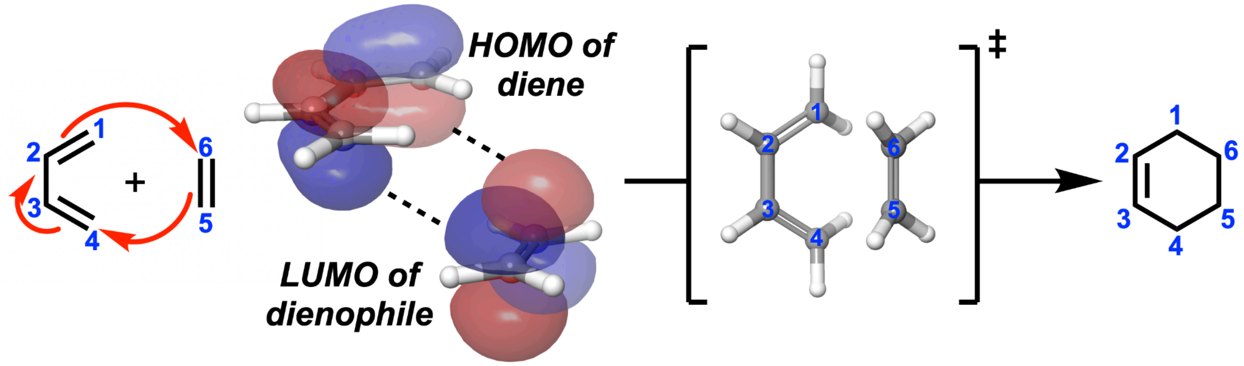
Diels-Alder Reactions



Diels-Alder Reactions

About this Lesson:

In this lesson plan, students will examine the relationship between a diene and a dienophile in a Diels-Alder reaction. Transition state theory will be introduced to analyze the concerted mechanism of a [4+2] cycloaddition. Reaction energy diagrams will be investigated to determine whether a reaction is exergonic or endergonic.

Using Maestro, students will use Jaguar's AutoTS panel to calculate the energetics of the reactants, product, and transition state. Students will also calculate the HOMO and LUMO of reactants to help with visualizing π molecular orbital overlap.

Learning Objectives:

- Identify transition state structures of Diels-Alder reaction mechanisms
- Plot reaction energy diagrams with activation energy barriers to determine their chemical reactivity characteristics (i.e. endergonic, exergonic, etc.)
- Generate molecular orbitals of the diene and dienophile to analyze favorable orbital overlap for product formation

Lesson Contents:

Standards Alignment:

- IB Diploma Programme:
    - What drives chemical reactions (Reactivity 1)
- ACS Guidelines
    - Substitution mechanisms (Conceptual Topics)
- AAMC MCAT
    - Structure, function, and reactivity of biologically-relevant molecules (5D)

Assessments for Understanding:

The following types of formative assessments are embedded in this lesson:

- Assessment of student understanding through discussion of warm-up questions and filling in any knowledge gaps about substituent effects of Diels-Alder reactions
- Visual assessment of student-generated transition state structures, reaction energy diagrams of Diels-Alder reactions, and molecular orbitals of the reactants

Associated Documentation Pages: AutoTS panel, Jaguar Geometry Optimization: The Basics

Warm-Up Questions:

Watch the Khan Academy videos on the Diels-Alder reaction.

1) Label the following substituents as either electron-withdrawing or electron-donating:
    a) –COOH
    b) –Me
    c) –OH
    d) –NO_2

1) To speed up a Diels–Alder reaction, what types of substituents should be placed on the diene and dienophile?

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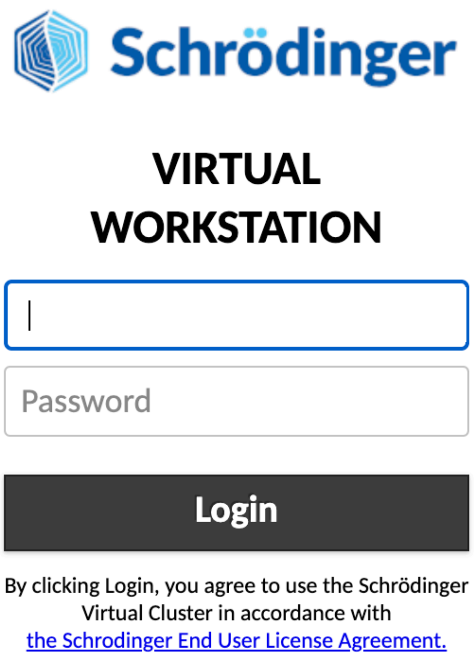
1. Setting Up the Maestro Session

At the start of the Maestro session, it is essential to 1) check your mouse actions, 2) change the file path to the Working Directory for this lesson, and 3) save your project file. The working directory indicated in this section contains the files necessary to complete this lesson. If you do not set the appropriate working directory, you will be unable to run any calculations.

1. Launch the Virtual Cluster



By clicking Login, you agree to use the Schrödinger Virtual Cluster in accordance with the Schrodinger End User License Agreement.

Figure 1-1. Virtual workstation login page.

2. Double-click the **course-data** folder on the desktop

Figure 1-2. Course-data folder on the desktop.

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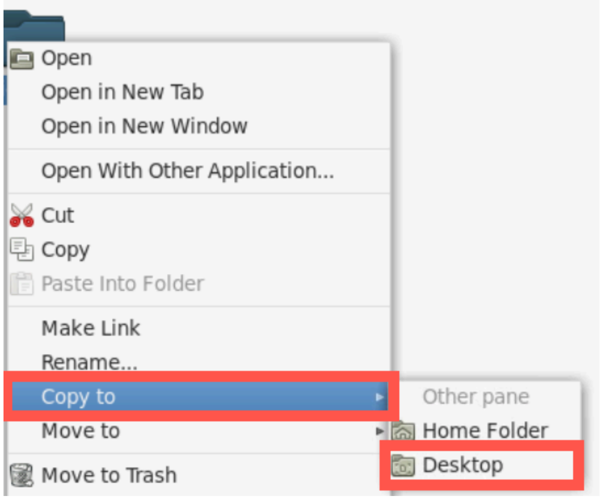
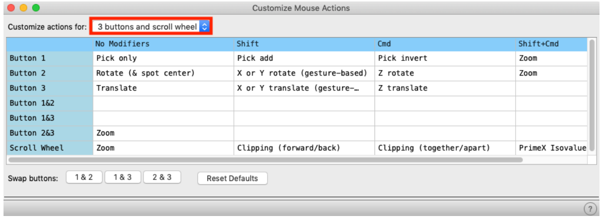


Figure 1-3. Copy the lesson folder to the Desktop.

3. Right-click the `Diels_Alder` folder and select **Copy to > Desktop**

4. Double-click the Maestro icon on the desktop



Customize actions for: 3 buttons and scroll wheel

	No Modifiers	Shift	Cmd	Shift+Cmd
Button 1	Pick only	Pick add	Pick invert	Zoom
Button 2	Rotate (& spot center)	X or Y rotate (gesture-based)	Z rotate	Zoom
Button 3	Translate	X or Y translate (gesture-…	Z translate	
Button 1&2				
Button 1&3				
Button 2&3	Zoom			
Scroll Wheel	Zoom	Clipping (forward/back)	Clipping (together/apart)	PrimeX Isovalue

Figure 1-4. Change the mouse actions.

5. Check your mouse actions.
    - Go to **Workspace > Customize Mouse Actions**
    - *Note:* This lesson was made with a three-button mouse with a scroll wheel, but a trackpad can still be used
    - ***Trackpad keys:***
        - **Up/Down trackpad** = Zoom In/Out
        - **Option** = Rotate
        - **Control** = Translate

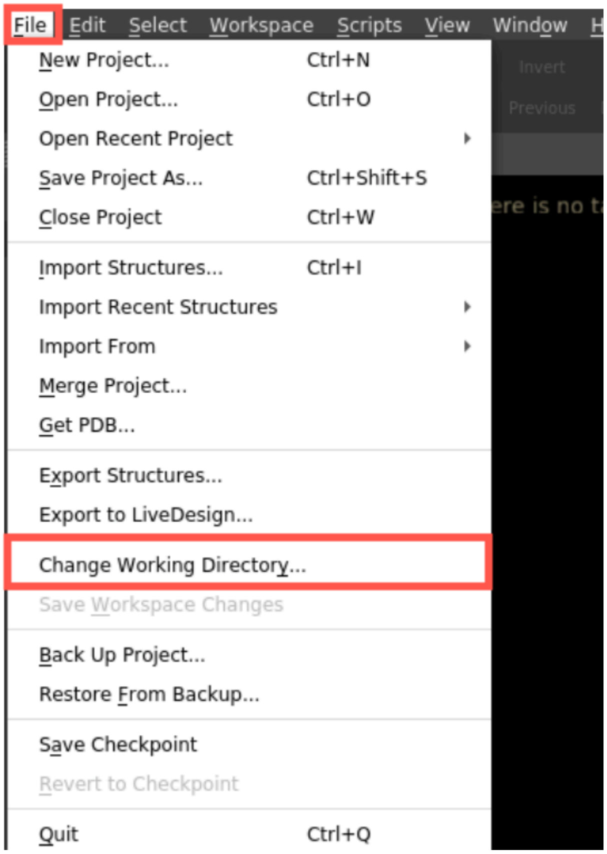
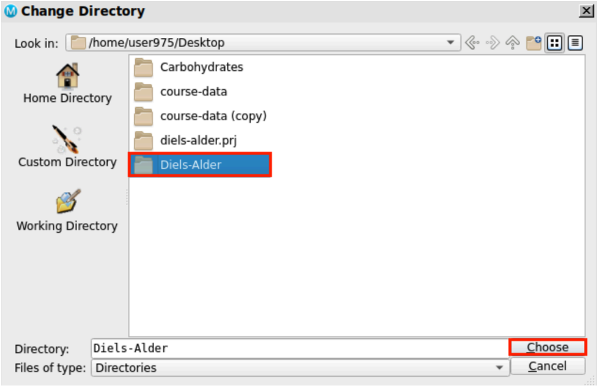


Figure 1-5. Change Working Directory option.

6. Go to File > Change Working Directory



Look in: /home/user975/Desktop

Directory: `Diels-Alder`

Files of type: Directories

Figure 1-6. Change Working Directory panel.

7. Navigate to Desktop > `Diels-Alder` folder and click **Choose**

Pre-generated input and results files are included for running jobs or examining output

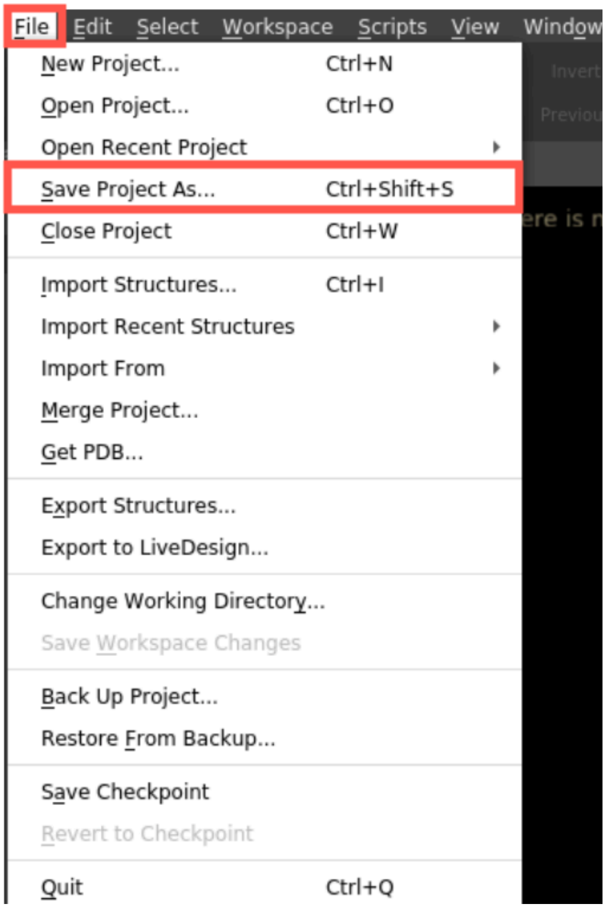
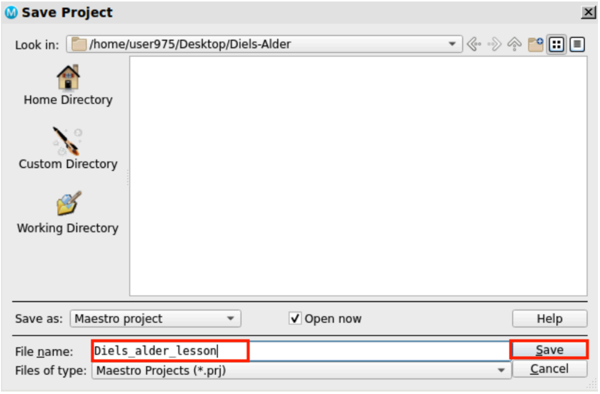


Figure 1-7. Save Project option.

8. Go to File > Save Project As



Look in: /home/user975/Desktop/Diels-Alder

Save as: Maestro project

☑ Open now

File name: Diels_alder_lesson

Files of type: Maestro Projects (*.prj)

Figure 1-8. Save Project panel.

9. Change the *File name* to `Diels_Alder_lesson`, click Save
    - The project is now named Diels_alder_lesson.prj

2. Introduction to Diels-Alder Reactions

The Diels-Alder reaction is a [4+2] cycloaddition that is part of a family of reactions called **pericyclic reactions**. In a pericyclic reaction, the two reactants are relatively non-polar and do not generally go through charged intermediates. A Diels-Alder reaction combines two components: a **diene** (a 4 π-electron component) and a **dienophile** (a 2 π-electron component). A **diene** is composed of two adjacent π bonds that are **conjugated**. A **dienophile** contains at least one π bond. In a Diels-Alder reaction, there is a pattern where 4 carbon atoms from the diene come together with 2 carbons from the dienophile to form a new 6-membered ring. The mechanism follows the same pattern where 3 C–C π bonds are broken, 2 new C–C bonds are formed, and a new C–C π bond is formed.

There are two ways to draw the arrow-pushing one-step, concerted mechanism of the Diels-Alder reaction: clockwise and counterclockwise. Both ways to depict the flow of electrons are correct and each way consists of drawing a total of 3 arrows. See **Figure 1** below for details:

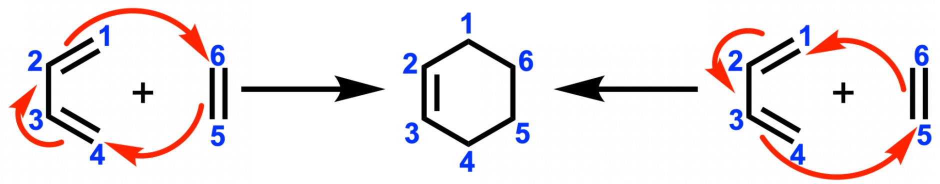
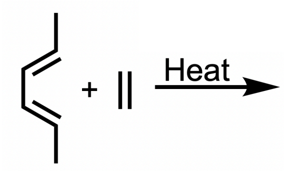


Figure 1. Concerted arrow-pushing mechanism for a Diels-Alder reaction

In a Diels-Alder reaction, the diene must be conjugated and in an *s*-cis conformation as shown above in **Figure 1**. Furthermore, substituents on either the diene or the dienophile do not affect the bond-forming and bond-breaking pattern in the reaction. Adding substituents to the reactants does however affect the reaction rate. It also affects the stereochemistry of the product which you can learn more about here. The rate of reaction is increased by electron-donating groups on the diene and electron-withdrawing groups on the dienophile.

For the scope of this lesson, it will only focus on normal electron demand Diels-Alder reactions, with an electron-rich diene and an electron-poor dienophile. However, there are examples of Diels-Alder reactions that proceed with electron-poor dienes and electron-rich dienophiles. Read more about inverse-electron demand Diels-Alder reactions here.

Practice #1. Predict the product and arrow-pushing mechanism of the following Diels-Alder reaction.



3. Generating Molecular Orbitals

Here we will show how the Diels-Alder reaction results form the constructive orbital overlap between the **highest occupied molecular orbital (HOMO)** of the diene with the **lowest unoccupied molecular orbital (LUMO)** of the dienophile. Since Diels-Alder reactions are concerted, multiple bonds are formed and broken at the same time, which means that *two* orbital interactions have to be considered. In order for the reaction to occur in a single step, there must be constructive overlap between each of the lobes where the bonds are being formed. If the phases are opposite, there is destructive interference between the orbitals which means there is zero electron density between the atoms. Visualizing the interactions between molecular orbitals is often difficult to see on paper, so we will calculate and generate molecular orbitals of the Diels-Alder reaction between butadiene and ethylene using Maestro's Jaguar.

Computational Exercise: Calculating Molecular Orbitals in Maestro

This exercise involves 3 parts:

Part 1: Build the molecules using 2D sketcher
Part 2: Run a Jaguar optimization job and calculate molecular orbitals
Part 3: Visualize the HOMO of the diene and LUMO of the dienophile

Part 1. Build reactants using 2D sketcher

Let's draw the structure of the reactants using the 2D sketcher.

1. Go to **Edit** > **2D Sketcher**

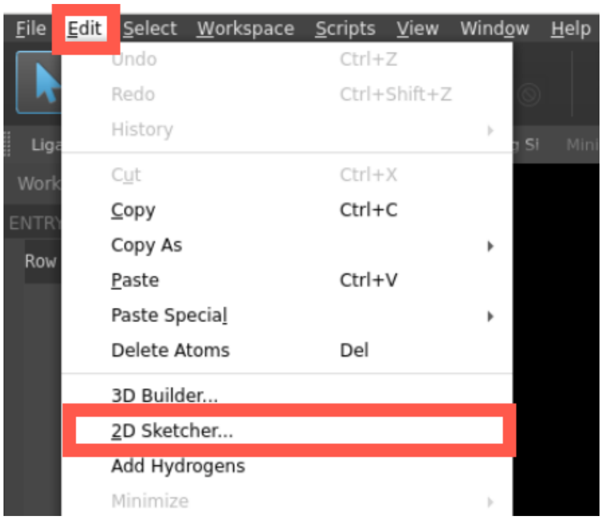
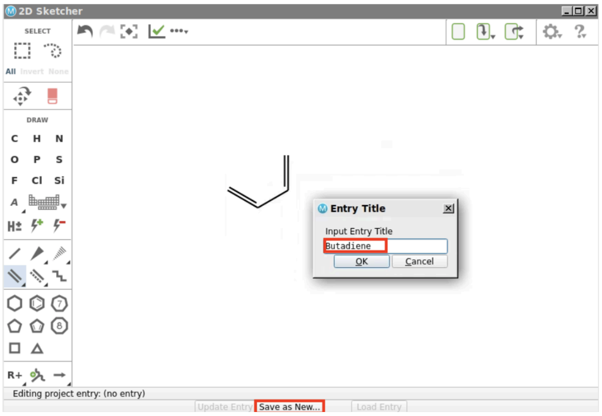


Figure 3-1. Open 2D Sketcher.



Butadiene

Figure 3-2. Drawing and saving butadiene.

2. **Draw** butadiene exactly how it is shown in Figure 2-2.
    - Go to the selection bar on the left
    - Select the single carbon bond button
    - Click and drag to add a carbon single bond. Continue to click and drag to draw a 4-carbon chain
    - Double click the single bond to add double bonds
    - Try to replicate the sketch shown in the figure as closely as possible
3. Click on **Save as New** and for *Input Entry Title* write **butadiene**. Click **OK**.
4. Check your structure to ensure it is in an *s*-cis conformation. If it is in *s*-trans, go to **Edit > 3D Builder**

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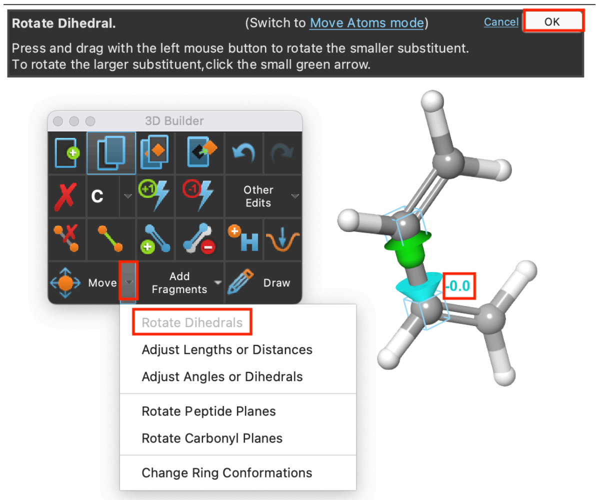

Rotate Dihedral. (Switch to Move Atoms mode) Cancel OK

Press and drag with the left mouse button to rotate the smaller substituent.
To rotate the larger substituent,click the small green arrow.

Figure 3-3. Changing the dihedral angle of s-trans butadiene to s-cis butadiene.

   - Click the dropdown arrow next to **Move**
   - Select **Rotate Dihedrals**
   - Adjust the C–C single bond dihedral angle to 0º
   - Click **OK** in the Rotate Dihedral banner

5. Repeat steps 1-3 to build the structure for ethylene

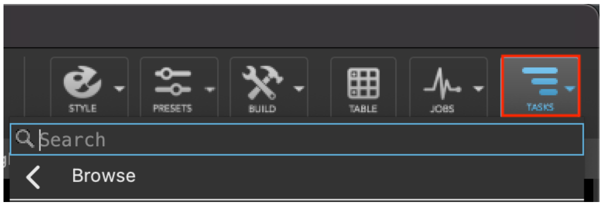
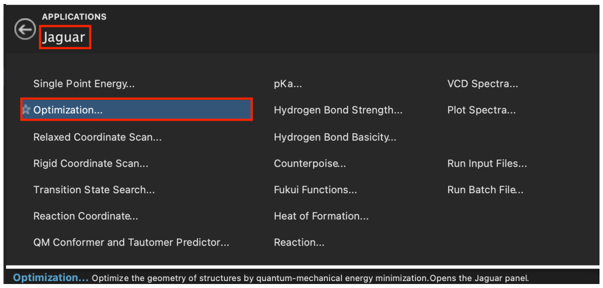
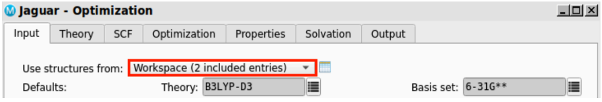


Figure 3-4. Clicking the Tasks button in the upper righthand corner.



Optimization... Optimize the geometry of structures by quantum-mechanical energy minimization.Opens the Jaguar panel.

Figure 3-5. Opening the Jaguar Optimization panel.



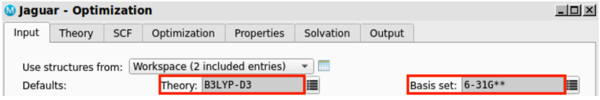
Use structures from: Workspace (2 included entries)
Defaults: Theory: B3LYP-D3 Basis set: 6-31G**

Figure 3-6. Setting the Jaguar Optimization panel to optimization.

Part 2. Optimize the Geometry using Quantum Mechanic DFT

Now let's optimize the molecule at the quantum mechanical level.

6. With both the butadiene and ethylene entries selected and included, go to **Tasks > Optimization** using Jaguar
   - The Jaguar Optimization panel opens
7. Use structures from **Project Table (2 selected entries)**



Use structures from: Workspace (2 included entries)

Defaults: Theory: B3LYP-D3 Basis set: 6-31G**

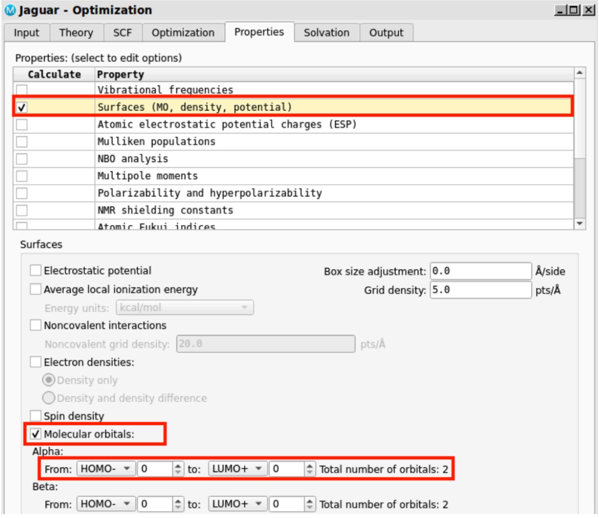
Figure 3-7. Setting the QM parameters for optimization.

Various settings can be altered depending on the specific use case. We will only adjust the *Input* tab for this example.

8. For *Theory*, select B3LYP-D3
9. For *Basis set*, select 6-31G**

A few additional comments about preparing for an optimization calculation:

- If you hover the mouse over the basis set in the table, you can see the number of basis functions associated with the basis set. This is useful to know since the quality of the basis set *usually* improves as the number of functions increases, noting again the trade-off between quality and computational expense
- Always make sure the charge and the spin multiplicity are correct (in this case, biphenyl is a neutral, singlet, so charge = 0 and spin multiplicity = 1). Multiplicity is defined as 2S + 1, where S is the total orbital spin of the molecule. For instance, a system with one unpaired electron is a doublet (multiplicity = 2), since the total orbital spin S = ½.
- Use the *Atom-Level Settings* button to define per-atom basis sets
- Constraints can be defined on the *Optimization* tab
- Properties, such as atomic charges, vibrational frequencies, surfaces and more can be requested on the *Properties* tab
- Solvent can be defined via several implicit solvation models on the *Solvation* tab. Note that this example is a gas-phase geometry optimization
- Read more about geometry optimization with Jaguar here



Jaguar - Optimization

Input | Theory | SCF | Optimization | Properties | Solvation | Output

Properties: (select to edit options)

Calculate	Property
☐	Vibrational frequencies
☑	Surfaces (MO, density, potential)
☐	Atomic electrostatic potential charges (ESP)
☐	Mulliken populations
☐	NBO analysis
☐	Multipole moments
☐	Polarizability and hyperpolarizability
☐	NMR shielding constants
☐	Atomic Fukui indices

Surfaces

☐ Electrostatic potential

Box size adjustment: 0.0 Å/side

☐ Average local ionization energy

Grid density: 5.0 pts/Å

Energy units: kcal/mol

☐ Noncovalent interactions

Noncovalent grid density: 20.0 pts/Å

☐ Electron densities:

● Density only

○ Density and density difference

☐ Spin density

☑ Molecular orbitals:

Alpha:

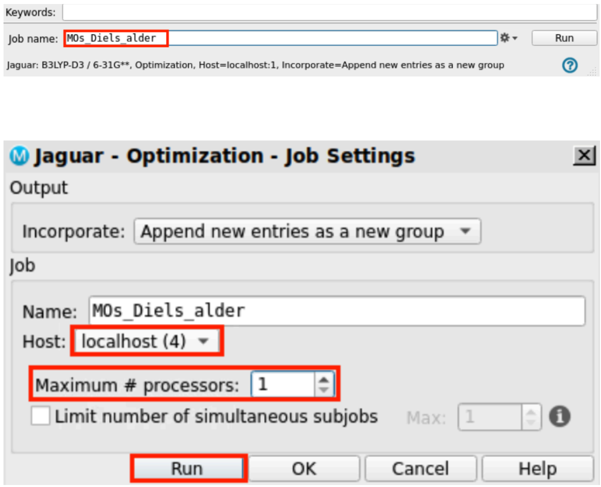
From: HOMO- 0 to: LUMO+ 0 Total number of orbitals: 2

Beta:

From: HOMO- 0 to: LUMO+ 0 Total number of orbitals: 2

Figure 3-8. Selecting MO Surfaces in the Properties Tab.

10. Go to the Properties Tab
11. Select *Surfaces (MO, density, potential)*
12. Check mark *Molecular orbitals*
13. Leave HOMO-0 and LUMO+0 for this exercise. If you would like to visualize more molecular orbitals, you may increase these values as necessary



Keywords:

Job name: MOs_Diels_alder

Jaguar: B3LYP-D3 / 6-31G**, Optimization, Host=localhost:1, Incorporate=Append new entries as a new group

Jaguar - Optimization - Job Settings

Output

Incorporate: Append new entries as a new group

Job

Name: MOs_Diels_alder

Host: localhost (4)

Maximum # processors: 1

☐ Limit number of simultaneous subjobs Max: 1

Figure 3-9. Naming and running the job.

14. Change the *Job name* to **MOs_Diels_alder**
15. Adjust the job settings by clicking the gear button to the right of the Job name
    - Choose localhost as your host with 1 processor
16. Click **Run**

Title Your job [redacted] has been incorporated. *1 min ago*

Figure 3-10. Banner that shows the job is finished – Result has been incorporated.

When the job finishes, a banner will appear indicating that the result has been incorporated. At this time, the molecules with the optimized geometries are now shown in the workspace.

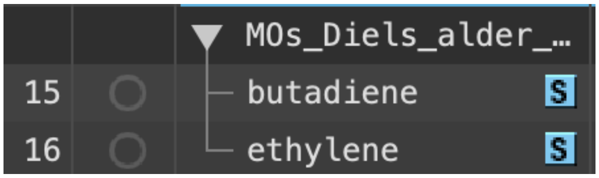

MOs_Diels_alder_…
15 ○ butadiene S
16 ○ ethylene S

Figure 3-11. The output molecules.

17. A new entry group is added to the entry list. Select and include the molecules titled butadiene and ethylene in this subgroup. These are your optimized structures.

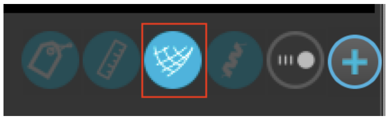


Figure 3-12. Toggling the surfaces on.

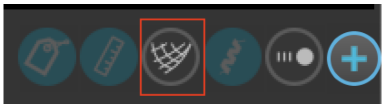


Figure 3-13. Toggling the surfaces off.

18. You can toggle on and off the molecular orbital surfaces at the bottom right-hand corner. Let’s turn it off for now.
19. Change the representation to ball-and-stick by clicking on the **Style** menu and choosing **Apply ball-and-stick representation**

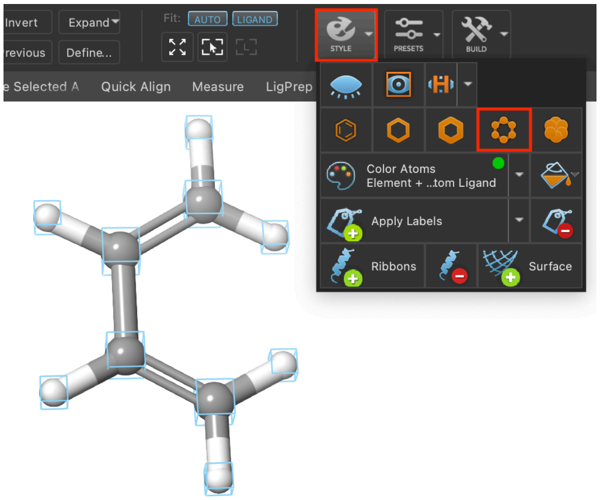


Figure 3-14. Viewing and styling butadiene and ethylene.

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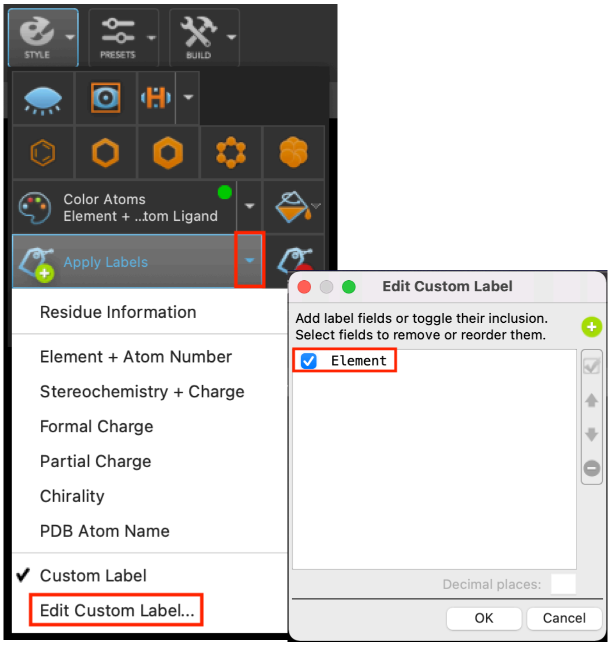


Add label fields or toggle their inclusion.
Select fields to remove or reorder them.

Figure 3-15. Labeling atoms.

20. To display atom labels, click **Style > Apply Labels** then click the drop down arrow on the right side
21. Click **Edit Custom Labeling**
22. Checkbox **Element** and press **OK**
23. Go back to **Style > Apply Labels > Custom Label** and now each atom in your workspace should be labeled

Note: You can toggle the atom labels on and off by clicking Annotations label button in the Workspace toggle on the bottom right corner

Figure 3-16. Toggling labels on.

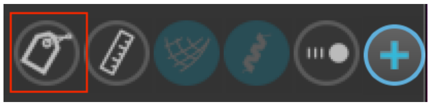


Figure 3-17. Toggling labels off.

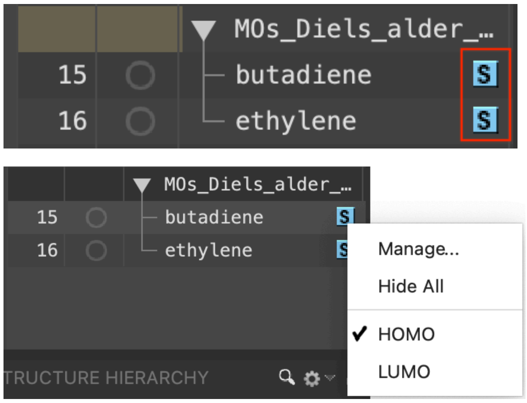


Figure 3-18. Selecting the Surface 'S' button in the Entry List

Part 3. Visualize the HOMO and LUMO

Now that we optimized the geometry of biphenyl, let's visualize the molecular orbitals.

24. Click the **S** button in the Entry List to the right of each entry
25. Select either the HOMO or the LUMO to visualize

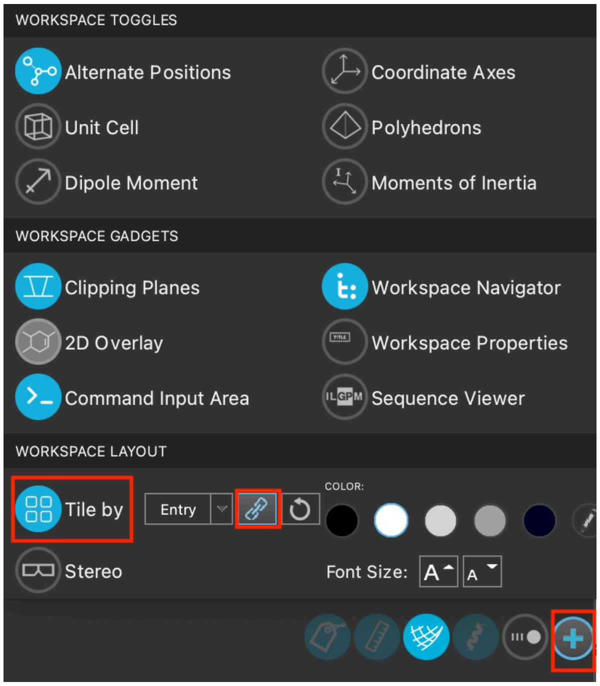


Figure 3-19. Tile the molecules side-by-side.

26. If you do not see any surfaces appear onto the molecule, remember to Toggle On the surfaces button in the bottom right-hand corner
27. Tile the 2 structures to visualize the MOs of the diene and dienophile side-by-side by selecting the **+** button in the bottom right-hand corner of the interface
28. Select the **Tile by** button under Workspace Layout
    - By default, moving the two molecules will be linked. If you wish to move only one molecule at a time, you can unlink their movement by deselecting the link button

Pause & Think #1. Take screenshots of the HOMO of the diene and the LUMO of the diene. Where does the orbital overlap occur between the two reactants?

4. Locating Transition States with AutoTS

Next, we are going to analyze the Diels-Alder reaction between butadiene and ethylene by determining the energetics of the reactants, transition state structure, and products. To do this, we will be using Maestro, Schrödinger's molecular modeling software.

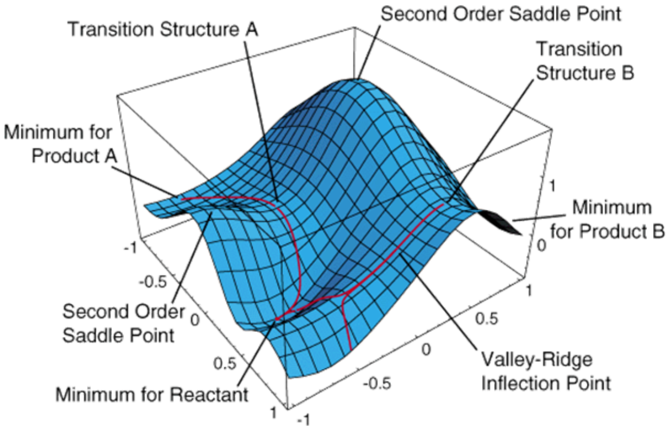


Figure 3.1. General potential energy surface.

Used with permission. Created by Professor H. Bernhard Schlegel, Wayne State University, Detroit, MI.

Locating a transition state is essential for computing the activation energy of a reaction, and thereby the reaction rate. As a result, finding transition states is useful in many applications: predicting reactivity, understanding reaction mechanisms, catalyst design and optimization, predicting outcomes of various competing reactions and more. Besides, locating a transition state is unique to computation -- meaning the transition state cannot be 'found' in the lab. Read more about Schrödinger's work in the space of Catalysis and Chemical Reactivity.

Searching for a transition state is typically a relatively difficult task in molecular modeling. Unlike an optimization to a minimum (see: Introduction to Geometry Optimizations, Functionals and Basis Sets), the search for a transition state highly depends on the quality of the initial guess, the initial Hessian and the search direction. Search for transition states is sometimes described as an 'art'. Experience and practice are key, as well as maintaining a thorough understanding of the available tools.

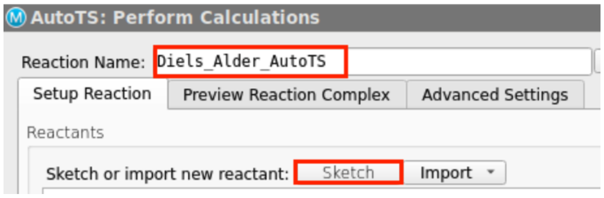
There are several alternative approaches to searching for a transition state with Jaguar (Schrödinger's Quantum Mechanics Engine). For this lesson, we will be using the AutoTS panel which is an automated workflow in which reactants and products are input and interpolation is used to search for the transition state with minimal user intervention. AutoTS is an automated way of finding transition states, particularly for elementary reactions. Its workflow requires only the structures of the reactants and the products as input, and then automates the rest of the process: it optimizes reactants and products, determines which bonds are breaking and forming, establishes correspondence between atoms in the reactants and the products, generates a transition state guess (either from a template or using an interpolated reaction path), launches a transition state search with the DFT engine Jaguar, verifies if the located transition state is trustworthy, runs frequency calculations, connects the transition state with the reactants and the products using an intrinsic reaction coordinate (IRC) algorithm and finally prints the potential energy surface diagram showing the transition state barrier. AutoTS works best on reactions that have only one transition state between the reactants and the products, such as the Diels-Alder reaction.

Computational Exercise #2: Generating a Transition State, Geometries of Reactants and Products, and an Energy Diagram using AutoTS

Let's employ the AutoTS panel for the Diels-Alder reaction between butadiene and ethylene. When an AutoTS job is submitted, it produces the following results:

1) Optimized geometries of the reactants and products

2) A transition state structure with an animation to show bonds breaking and forming
3) A potential energy surface diagram that includes a transition state barrier



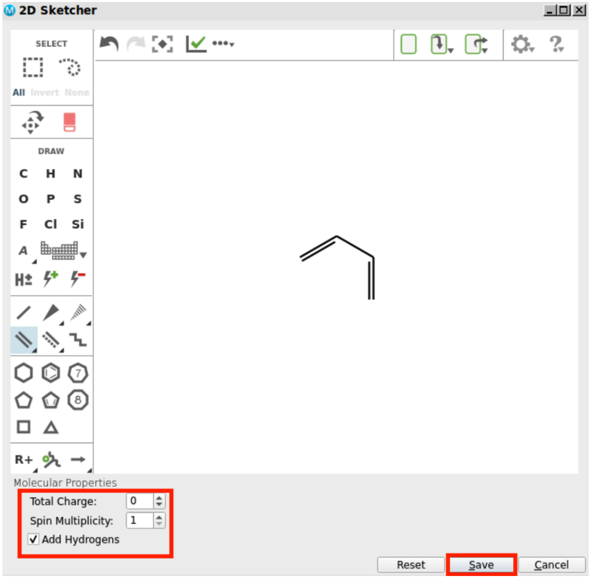
AutoTS: Perform Calculations

Reaction Name: Diels_Alder_AutoTS

Figure 4-1. Opening the AutoTS panel.

We will first perform an AutoTS calculation on a simple Diels-Alder reaction between chloroethane and a bromide ion to learn the mechanics of the panel.

1. Go to **Tasks** and type **AutoTS**. Click **AutoTS... Other Applications** (under the AutoTS category)
    - The AutoTS: Perform Calculations panel opens
2. Change the Reaction Name to **Diels_Alder_AutoTS**



Total Charge: 0

Spin Multiplicity: 1

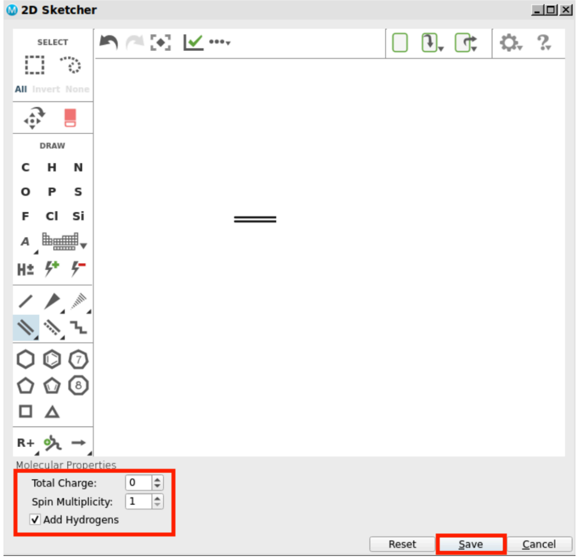
☑ Add Hydrogens

Figure 4-2. Sketching the butadiene reactant in the AutoTS panel.

3. Under *Reactants*, click **Sketch** and **draw butadiene**. In the 2D Sketcher, select the carbon single bond, then click and drag to form a C–C single bond, and continue adding to get a 4-carbon chain. Under Molecular Properties, ensure the Total Charge is 0, Spin Multiplicity is 1, and the box to Add Hydrogens is checked. It’s okay if butadiene appears to be *s*-trans in the AutoTS panel – it will reorient to *s*-cis during geometry optimization. Click **Save**.
4. Under *Reactants*, click **Sketch** and **draw ethylene.** In the 2D Sketcher,

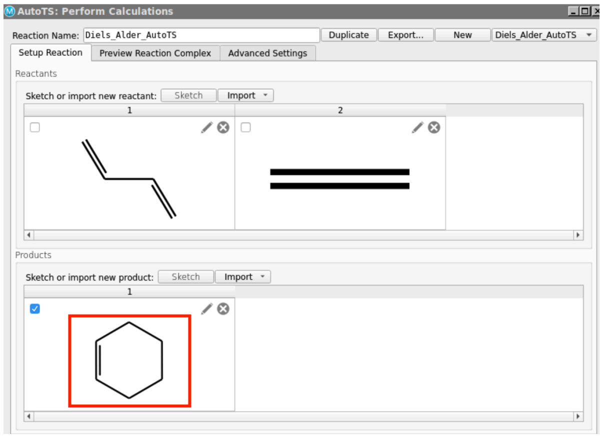
select the carbon single bond, then click and drag to form a C–C single bond, and double-click to form a double bond. Under Molecular Properties, ensure the Total Charge is 0, Spin Multiplicity is 1, and the box to Add Hydrogens is checked. Click **Save**.

5. Under *Products*, repeat the process and draw the products of the Diels-Alder reaction.
    - Your inputs should match the *Figure 6-4.*



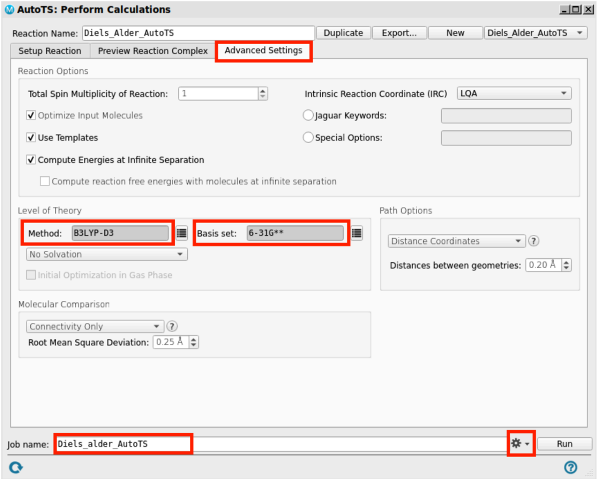
Total Charge: 0
Spin Multiplicity: 1
☑ Add Hydrogens

Figure 4-3. Sketching the Cl^- reactant in the AutoTS panel.



Reaction Name: Diels_Alder_AutoTS

Figure 4-4. Sketching the products in the AutoTS panel.



AutoTS: Perform Calculations

Reaction Name: Diels_Alder_AutoTS

Reaction Options

Total Spin Multiplicity of Reaction: 1

Intrinsic Reaction Coordinate (IRC): LQA

☑ Optimize Input Molecules

○ Jaguar Keywords:

☑ Use Templates

○ Special Options:

☑ Compute Energies at Infinite Separation

☐ Compute reaction free energies with molecules at infinite separation

Level of Theory

Method: B3LYP-D3

Basis set: 6-31G**

No Solvation

☐ Initial Optimization in Gas Phase

Path Options

Distance Coordinates

Distances between geometries: 0.20 Å

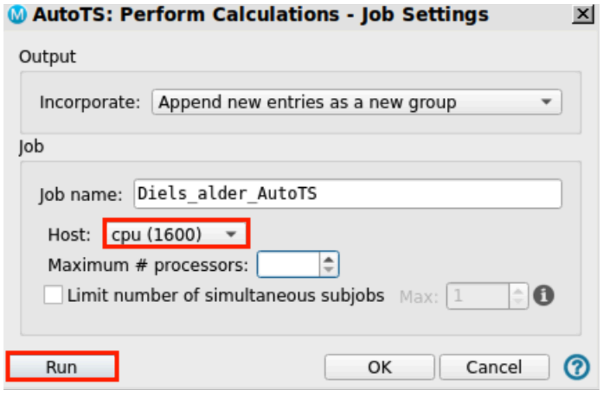
Molecular Comparison

Connectivity Only

Root Mean Square Deviation: 0.25 Å

Job name: Diels_alder_AutoTS

Figure 4-5. Advanced settings and naming the job.



AutoTS: Perform Calculations - Job Settings

Output

Incorporate: Append new entries as a new group

Job

Job name: Diels_alder_AutoTS

Host: cpu (1600)

Maximum # processors:

☐ Limit number of simultaneous subjobs Max: 1

Figure 4-6. Adjusting job settings from the gear icon and running the job.

6. Go to the **Advanced Settings** tab
    - ○ We will keep the settings as default in this case
    - ○ Level of theory:
        - i. Method: B3LYP-D3
        - ii. Basis Set: 6-31G**
7. Change the *Job name* to **Diels_Alder_AutoTS**
8. Adjust the job settings (⚙▾) as needed
    - ○ Change host from local host to **CPU host**.
    - ○ Change the **Maximum # of Processors to 12**. The job can be completed in about 5 minutes on a 12 CPU host
9. If you would like to run the job yourself, click **Run**. Otherwise, we can import pre-generated outputs in the analysis stages
10. **Close** the AutoTS panel

Note: The *Preview Reaction Complex* tab can be used to generate reactant and product complexes (merged structures) and to see a guess at the reaction path. Adjustments can be made as needed

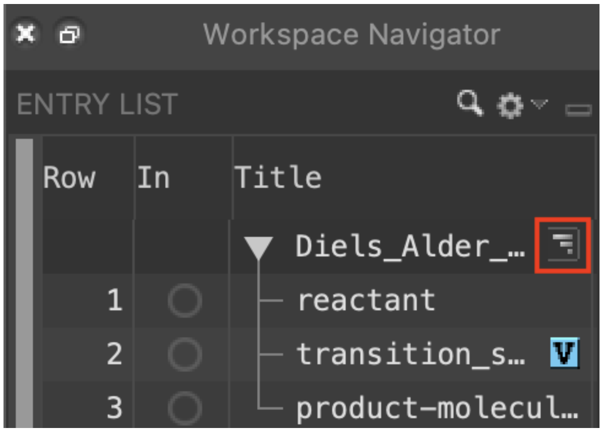


Figure 4-7. Importing the results of the AutoTS calculation.

When the job is complete, we can view the results in the AutoTS: View Results panel. The AutoTS calculation assesses various paths without any additional user input

11. Go to **File > Import Structures**
12. Select the Diels_Alder_AutoTS_full_path.mae file and click **Open**
    - If you did not perform the calculation yourself and wish to open the pre-generated results, select the Diels_Alder_AutoTS_full_path.mae file and click **Open**
    - An entry group including the reactant, transition state and product structures is added to the entry list
13. Use the Workflow Action Menu (WAM) button (▤) to access the Results panel

Alternatively, go to **Tasks** and type **AutoTS Results** and load the full_path.mae file via the **Import** button

Figure 4-8. AutoTS results.

The AutoTS: View Results panel contains the energy diagram associated with the reaction. If you are interested in viewing the vibration associated with the transition

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	state, use the vibration viewer (V) in the entry list and animate in the workspace

Pause & Think #2. Using the AutoTS results, let's analyze the Diels-Alder reaction further. Answer the following questions:

a) Take screenshots of the optimized geometries for the reactants, transition state structure, and products.
b) List the C–C bond distances of each molecule using the Measure button in units of ångstroms.

Reactants	Transition State Structure	Products
Screenshot:	Screenshot:	Screenshot:
Bond distances:	Bond distances:	Bond distances:

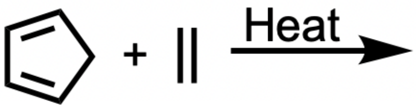
c) Now let’s analyze the transition state structure. Look at the animation of its vibration. What is the hybridization of the carbon atoms involved in the bond breaking and forming at the transition state? How does this differ from the reactants’ starting geometry?

d) Take a screenshot of the reaction energy diagram. Is the reaction exergonic or endergonic? What is the activation energy barrier in units of kcal/mol? Would the reaction speed up or slow down if the dienophile included an electron-withdrawing group such as an aldehyde?

5. Individual Exercise

Part A:

For the following Diels-Alder reaction:



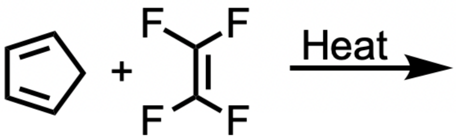
1) Label which reactant is the diene and which is the dienophile. Then, predict the product and draw the arrow-pushing mechanism.

2) Generate the HOMO and LUMO of the diene and dienophile. Take a screenshot and paste it below.

HOMO of Diene	**LUMO of Dienophile**

Part B:

For the following Diels-Alder reaction:



1) Label which reactant is the diene and which is the dienophile. Then, predict the product and draw the arrow-pushing mechanism.

2) Look at the pre-generated AutoTS results for this reaction. Take screenshots of the optimized geometries for the reactants, transition state structure, and products.

Reactants	Transition State Structure	Products
Screenshot:	Screenshot:	Screenshot:

3) Take a screenshot of the reaction energy diagram. Is the reaction exergonic or endergonic? What is the activation energy barrier in units of kcal/mol?

Part C:

Compare the two reactions from Part A and Part B. Which reaction do you expect to have a faster reaction rate and why?

7. Summary, Additional Resources, and References

Using Maestro, students learned how to use Jaguar's AutoTS panel to perform geometry optimization calculations of the reactants and products of a Diels-Alder reaction, determine which bonds are breaking and forming, establish correspondence between atoms in the reactants and the products, and generate a transition state structure.They learned how to render a potential energy surface diagram to show the activation energy barrier. Lastly, students generated molecular orbitals of the diene and dienophile to better understand that constructive orbital overlap is necessary for new bond formation..

For further learning:

For introductory content, focused on navigating the Schrödinger Materials Science interface, an Introduction to Maestro for Materials Science tutorial is available.

For some related practice, proceed to explore other relevant tutorials:

- Introduction to Geometry Optimizations, Functionals, and Basis Sets
- Locating Transition States

For further reading:

- Introduction to Computational Chemistry, 3rd Edition
- Essentials of Computational Chemistry: Theories and Models, 2nd Edition
- See the Jaguar help documentation

8. Glossary of Terms

Entry List - a simplified view of the Project Table that allows you to perform basic operations such as selection and inclusion

Included - the entry is represented in the Workspace, the circle in the In column is blue

Project Table - displays the contents of a project and is also an interface for performing operations on selected entries, viewing properties, and organizing structures and data

Recent actions - This is a list of your recent actions, which you can use to reopen a panel, displayed below the Browse row. (Right-click to delete.)

Scratch Project - a temporary project in which work is not saved. Closing a scratch project removes all current work and begins a new scratch project

Selected - (1) the atoms are chosen in the Workspace. These atoms are referred to as "the selection" or "the atom selection". Workspace operations are performed on the selected atoms. (2) The entry is chosen in the Entry List (and Project Table) and the row for the entry is highlighted. Project operations are performed on all selected entries

Working Directory - the location that files are saved

Workspace - the 3D display area in the center of the main window, where molecular structures are displayed

2D Workspace - the 2D panel that opens from the “edit” dropdown that allows for the construction of molecules using a 2D sketcher

Tile - if multiple entries are included, included entries are displayed side by side in individual boxes rather than being overlaid in the same space