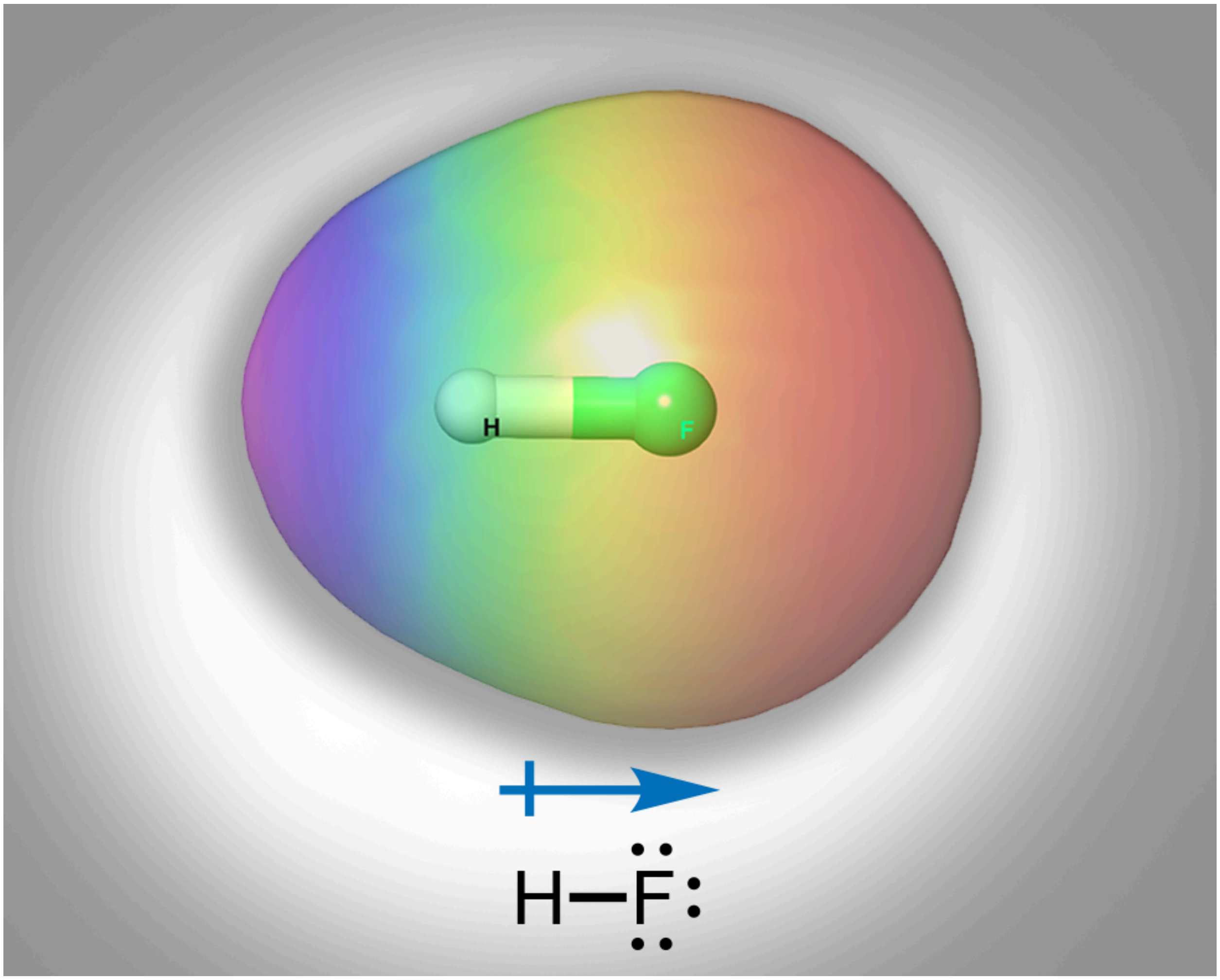
Chemical Bonding



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Chemical Bonding

About this Lesson:

In this lesson, students will examine the relationship between the electronic structure of atoms and the ionic and covalent chemical bonds they form. Students will learn about bond polarity and electronegativity by looking at electron distributions of various small molecules.

Using Maestro, students will create a map of electrostatic potential (ESP) of various small molecules with Jaguar and examine the electrostatic potential on the molecular surface. These renderings will help with visualizing electronegativity trends and gauging the polarity of chemical bonds.

Learning Objectives:

- Explain the relationship between the type of bonding and the properties of the elements participating in the bond.
- Use electronegativity differences to identify nonpolar covalent, polar covalent, and ionic bonds.
- Identify a chemical bond type by mapping electrostatic potential surfaces onto molecules.

Lesson Contents:

1. Setting Up the Maestro Session
2. Lewis Electron-Dots
3. Ionic Bonding
4. Covalent Bonding
5. Bond Polarity and Electronegativity
6. Individual Exercises
7. Summary, Additional Resources, and References
8. Glossary of Terms

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Standards Alignment:

- *Connections to AP*
    - ○ Models and Representations (Skill 1)
- *IB Diploma Programme:*
    - ○ Models of bonding and structure (Structure 2)
- *ACS Guidelines*
    - ○ Understand molecular structure and bonding (Coursework Guidelines)
- *AAMC MCAT*
    - ○ Nature of molecules and intermolecular interactions (5B)

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 chemical bond types
- Visual assessment of student-generated electrostatic potential maps

Associated Documentation Pages: Jaguar Geometry Optimization: The Basics

Warm-Up Questions:

Watch the Khan Academy videos on molecular and ionic compound structure and properties.

1. Using Lewis symbols, diagram the reaction between magnesium and oxygen atoms to give the ionic substance MgO.
2. How many electrons are transferred?
3. Which atom loses electrons in the reaction?

Need help? Contact us at teaching@schrodinger.com

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

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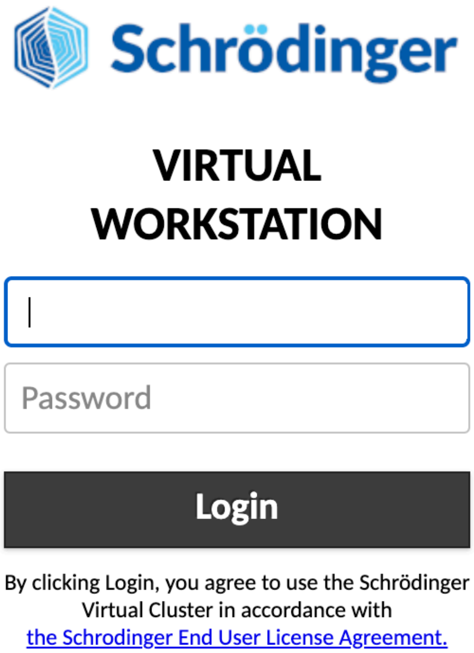
lesson. If you do not set the appropriate working directory, you will be unable to run any calculations.

1. Launch the Virtual Cluster



Schrödinger

VIRTUAL WORKSTATION

Password

Login

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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Back to Lesson Contents

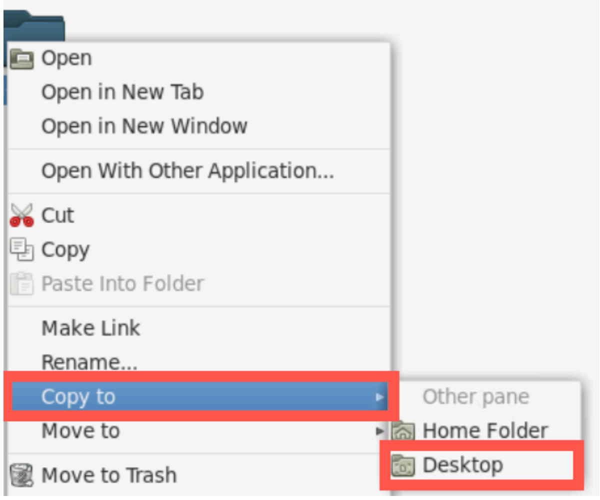
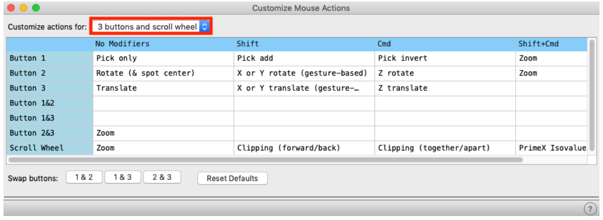


Figure 1-3. Copy the lesson folder to the Desktop.

3. Right-click the `chemical_bonding` 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

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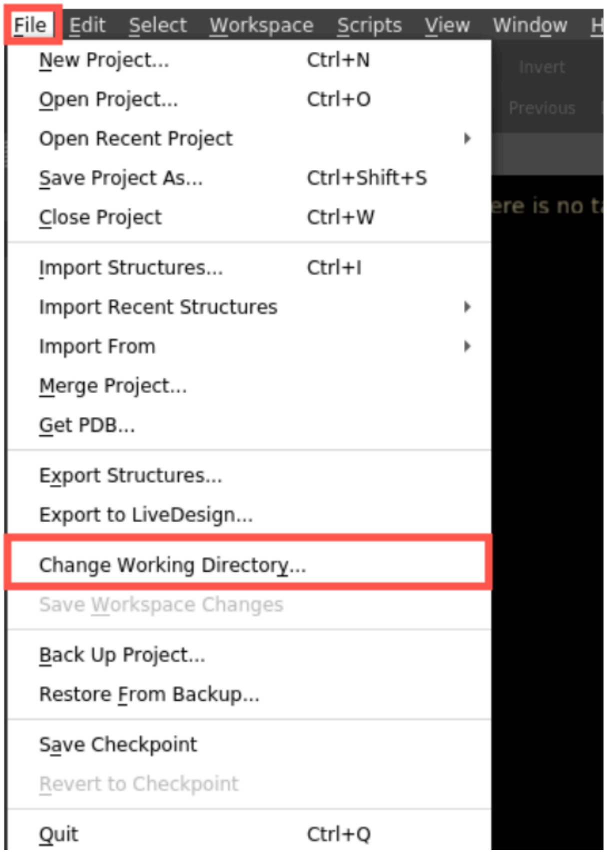
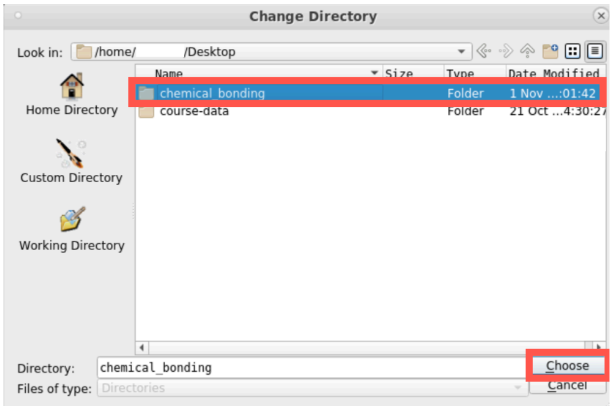


Figure 1-5. Change Working Directory option.

6. Go to File > Change Working Directory



Look in: /home/ /Desktop

Name	Size	Type	Date Modified
chemical_bonding		Folder	1 Nov ...:01:42
course-data		Folder	21 Oct ...4:30:2

Directory: chemical_bonding

Files of type: Directories

Figure 1-6. Change Working Directory panel.

7. Navigate to Desktop > `chemical_bonding` folder and click **Choose**

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

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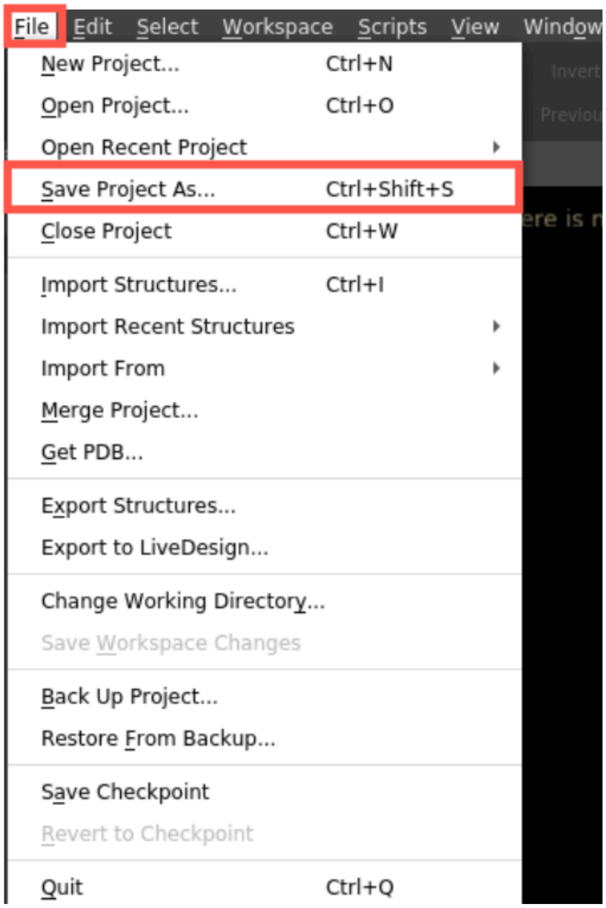
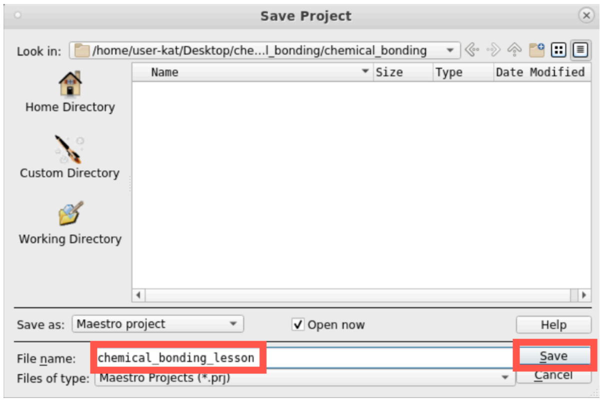


Figure 1-7. Save Project option.

8. Go to File > Save Project As



Look in: /home/user-kat/Desktop/che...l_bonding/chemical_bonding

Save as: Maestro project

☑ Open now

File name: chemical_bonding_lesson

Files of type: Maestro Projects (*.prj)

Figure 1-8. Save Project panel.

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

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2. Lewis Electron Dots

Electrons involved in chemical bonding are called ***valence electrons***, which are located in the outermost occupied shell. A simple way to show valence electrons in an atom is called a ***Lewis electron-dot symbol*** or a ***Lewis symbol***. A Lewis symbol for an element is made by placing dots representing valence electrons around the symbol for a particular element. For many common elements, the number of dots corresponds to the element's group number. For example, sulfur's electron configuration is [Ne]$3s^2 3p^4$ and contains six valence electrons. Therefore, the Lewis symbol for sulfur is

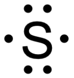

Figure 2-1. Sulfur's Lewis symbol

Notice that the dots are placed around the four sides of the element symbol – top, bottom, left, and right – and each side can hold up to two valence electrons. All four sides are equal, which means that the placement of lone pairs of electrons vs. single electrons is arbitrary. Generally, however, it is good practice to spread out the dots as much as possible. It is better to have two pairs of electrons and two single electrons, in sulfur's case, as opposed to three pairs of electrons, one single electron, and an empty side.

Atoms typically gain, lose, or share electrons to achieve the same number of electrons as the noble gas closest to them in the periodic table. The ***octet rule*** states that atoms tend to form compounds in ways that give them eight valence electrons, which is the electron configuration of a noble gas. In a Lewis symbol, an octet is shown as four pairs of valence electrons arranged around the element symbol. Although there are exceptions to the octet rule, we won't be covering them in this lesson plan. See this article for more information.

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Practice #1. Draw the electron configuration and Lewis electron dot symbol for the following elements listed in the table below.

Element	Electron Configuration	Lewis Symbol
Lithium		
Carbon		
Nitrogen		
Aluminum		
Chlorine		

3. Ionic Bonding

Ionic compounds are formed by the interaction of metals on the left side of the periodic table with nonmetals on the right side, excluding noble gasses in group 8A. Ionic compounds contain several characteristic properties. For instance, they are usually crystalline and are easy to break apart along smooth surfaces. Such characteristics result from the electrostatic forces that maintain the ions in a rigid, well-defined, three-dimensional arrangement. Ionic compounds are stable due to the attraction between ions of opposite charges. This attraction draws the ions together, releasing energy and causing the ions to form a solid lattice. Shown below is a crystal structure of sodium chloride (NaCl):

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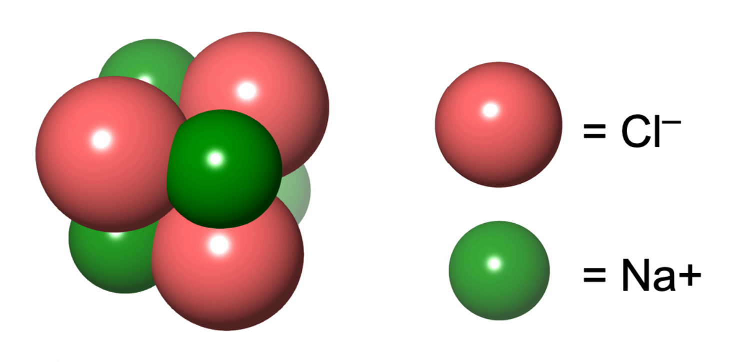

Figure 3-1. Crystal structure of sodium chloride in bulk

The formation of Na^+ from Na and Cl^- from Cl_2 indicates that an electron has been lost by a sodium atom and gained by a chlorine atom – an ***electron transfer*** from the Na atom to the Cl atom occurred. Recall that ***ionization energy*** indicates how easily an electron can be removed from an atom whereas ***electron affinity*** measures how much an atom wants to gain an electron. See here for more information. Electron transfer to form oppositely charged ions occurs when one atom readily gives up an electron (low ionization energy) and another atom readily gains an electron (high electron affinity). NaCl is a typical ionic compound because it consists of a metal, sodium, of low ionization energy and a non-metal, chlorine, of high electron affinity. The ionic bonding of NaCl can be represented using Lewis electron-dot symbols shown below.

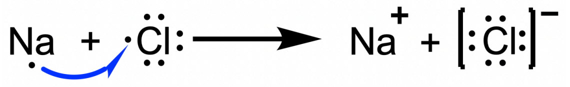

Figure 3-2. Lewis electron-dot symbols of the ionic bonding in NaCl

When oppositely charged particles, like Na^+ and Cl^-, attract to one another, this attractive force is referred to as an ***electrostatic force***. An ionic bond is the electrostatic force that holds the ions, Na^+ and Cl^-, together in an ionic compound. It's conventional to show the cation, Na^+, without dots around the symbol to emphasize that the original energy level that contained the valence electron is now empty. The anion, Cl^-, is now shown with a complete octet of electrons.

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4. Covalent Bonding

In ionic compounds, electrons are transferred between atoms of different elements to form ions. But this is not the only way that compounds can be formed. A chemical bond formed by sharing a pair of electrons is a ***covalent bond***. Covalent bonds are formed between two atoms when both have similar tendencies to attract electrons to themselves (i.e. when both atoms have identical or daily similar ionization energies and electron affinities).

Compounds that contain covalent bonds exhibit different physical properties than ionic compounds. Because the attraction between electrical neutral atoms is weaker than that between electrically charged ions, covalent compounds generally have much lower melting and boiling points than ionic compounds.

Previously you learned that the valence electrons of a single atom can be easily shown by a Lewis electron-dot symbol. The structures of molecules that are held together by covalent bonds can be diagrammed by ***Lewis electron-dot structures***, or ***Lewis structures*** for short. The simplest example of a covalent bond is the hydrogen molecule, H_2. Each hydrogen atom acquires a second electron, achieving the stable, two-electron, noble-gas configuration of helium. The two electrons in between each hydrogen atom are shared and are called a ***pair of bonding electrons***, or a ***single covalent bond***. A Lewis structure of H_2 is shown below where the single covalent bond can be shown by either the lone pair or as a dash in between the two atoms.

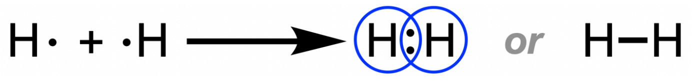

Figure 4-1. Lewis structure of H_2

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How to Draw Lewis Structures

Step #1: Add up all the valence electrons from all atoms, taking into account overall charge

- The number of valence electrons can be found from the periodic table
    - Ex. Carbon is in group 4A so it has 4 valence electrons
- For an anion, add one electron to the total for each negative charge
- For a cation, subtract one electron from the total for each positive charge

Step #2: Write the symbols for the atoms, show which atoms are attached to which, and connect them with single bonds (aka a line that represents two bonding electrons)

Step #3: Complete the octets around all the atoms bonded to the central atom

- Remember that a hydrogen atom only has a single pair of electrons around it

Step #4: Place any leftover electrons around the central atom

Step #5: If there are not enough electrons to give the central atom an octet, try multiple bonds (double or triple bonds)

Practice #2. Draw the Lewis structure for phosphorus trichloride, PCl_3 and show your work after each of the five steps.

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Computational Exercise #1: Geometry Optimization using Maestro

Although the Lewis structure of PCl_3 looks relatively flat and two-dimensional, now we are going to learn how to build a three-dimensional structure of PCl_3 and then optimize its geometry using Maestro. Visualizing the molecular structure can be done in three different ways:

1) Through the 2D Sketcher
2) Through the 3D Builder
3) Or, by importing pre-built molecules

We will be using the 2D Sketcher tool in Maestro.

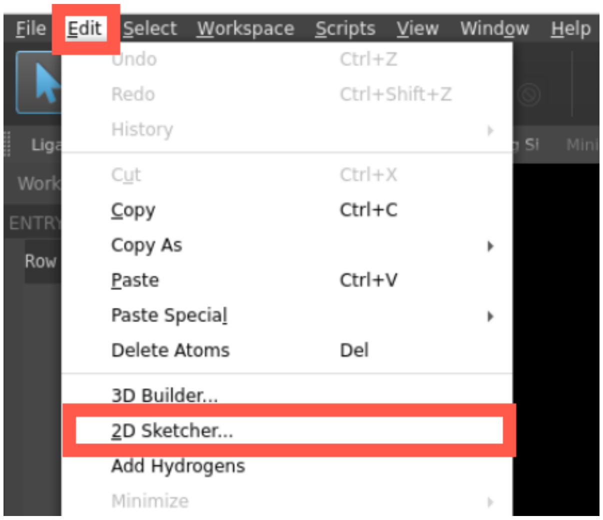

Figure 4-1. Open 2D Sketcher.

Part 1. Build PCl_3 using 2D Sketcher

Before optimizing any molecular geometry, you will need a starting molecule in your workspace. Let's draw the structure of PCl_3 using the 2D sketcher.

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

The 2D sketcher functions like many standard 2D molecular drawing tools. For a complete overview of using the sketcher panel, see the [2D Sketcher Panel documentation].

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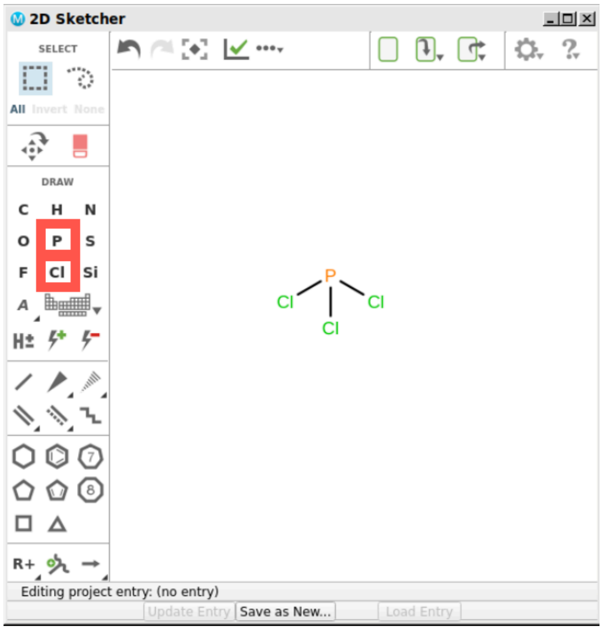
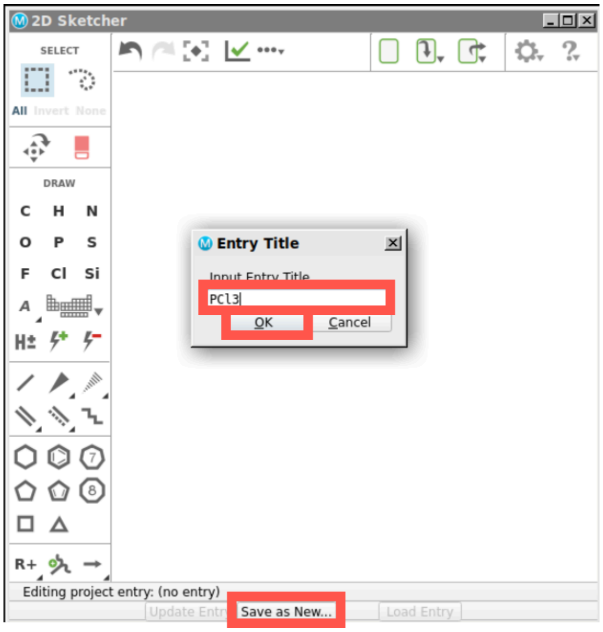


Editing project entry: (no entry)

Figure 4-2. Draw phosphorus trichloride, PCl_3.

Here, you will draw your Lewis Structure final answer of PCl_3. You do not need to draw in any lone pair of electrons; only show the bonds.

2. Go to the selection bar on the left
3. Choose the phosphorus atom "P" and click anywhere in the 2D Workspace to place
4. Choose the chlorine atom "Cl" and click and drag off of the "P" atom to create 3 P–Cl single bonds



Input Entry Title: PCl3

Editing project entry: (no entry)

Figure 4-3. Save the entry title for PCl_3.

5. Click on **Save as New**
6. For *Input Entry Title*, write **PCl3**.
7. Click **OK**.

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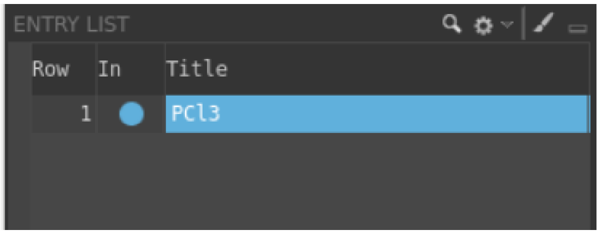

Row	In	Title
1	●	PCl3

Figure 4-4. Include and select the entry.

8. Close the 2D Sketcher panel
9. In the Entry List, ensure that the PCl_3 molecule is <u>selected</u> and <u>included</u> in the <u>workspace</u>

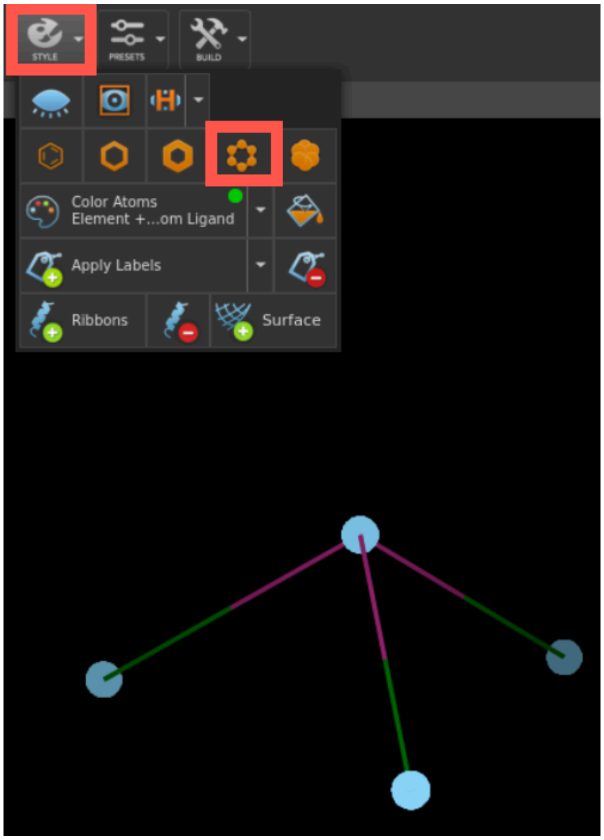

Figure 4-5. Viewing and styling PCl_3.

10. Change the representation to ball-and-stick by clicking on the **Style** menu and choosing **Apply ball-and-stick representation**

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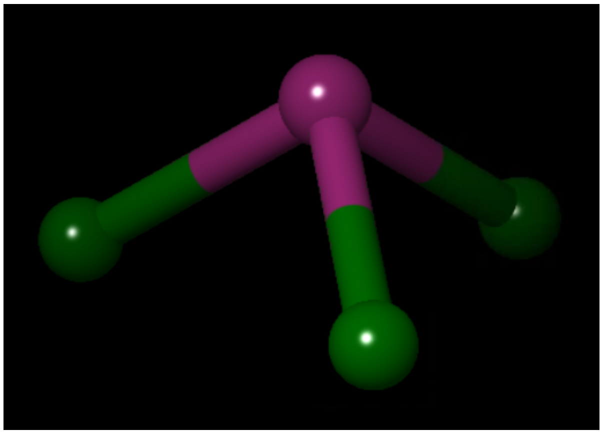

Figure 4-6. Styling PCl3 as ball-and-stick.

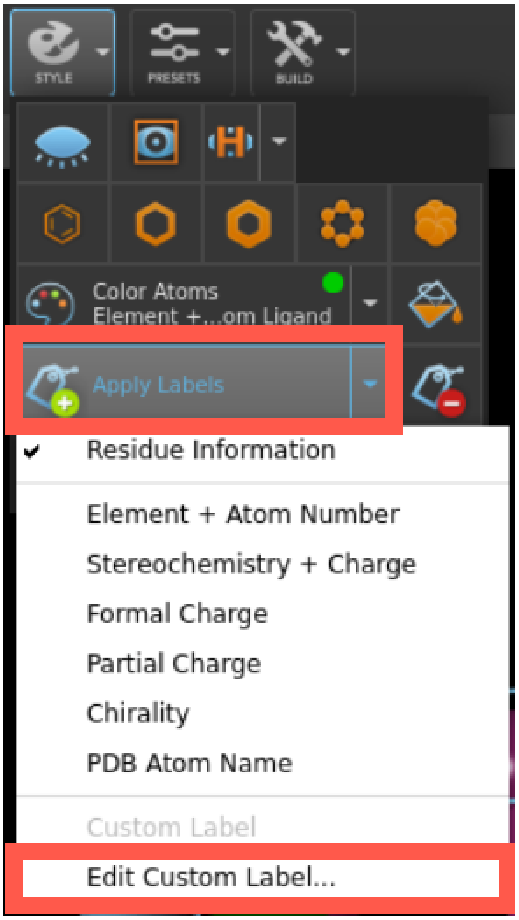

Figure 4-7. Labeling atoms.

11. To display atom labels, click **Style > Apply Labels > Edit Custom Label...**

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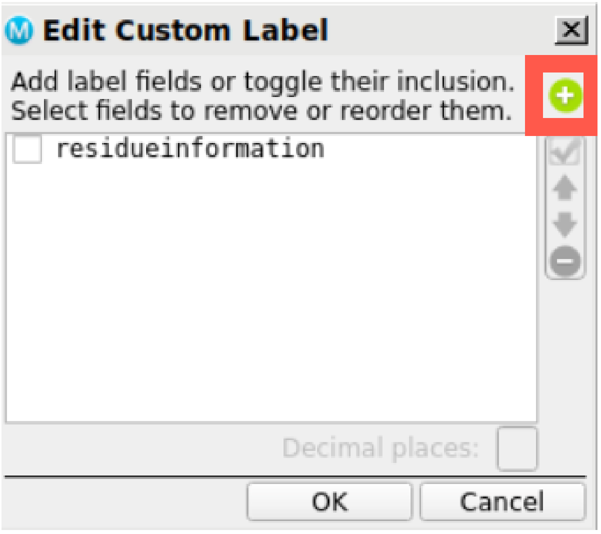

Figure 4-8. Editing custom labels.

12. The **Edit Custom Label** window will open
13. Click the green **plus** button

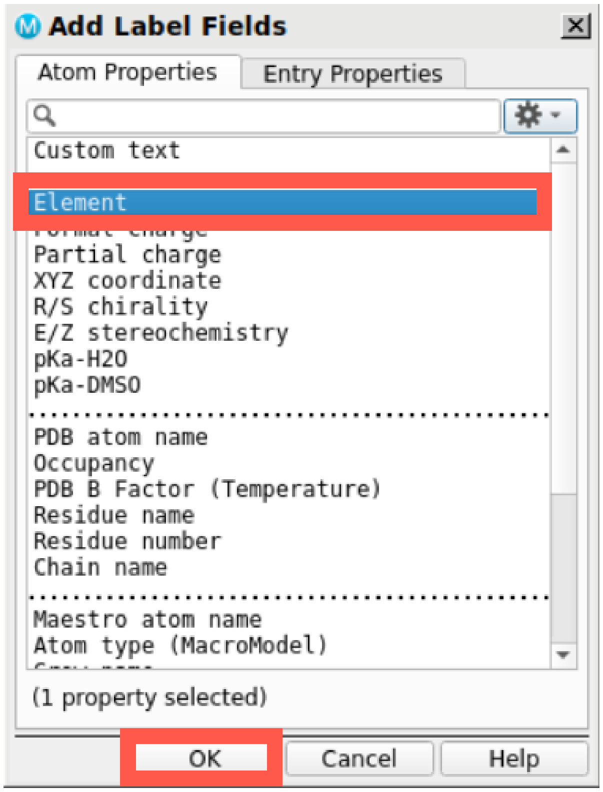

Figure 4-9. Adding label fields.

14. The **Add Label Fields** window will open
15. Select **Element** and press **OK**
16. In the **Edit Custom Label** window, press **OK**

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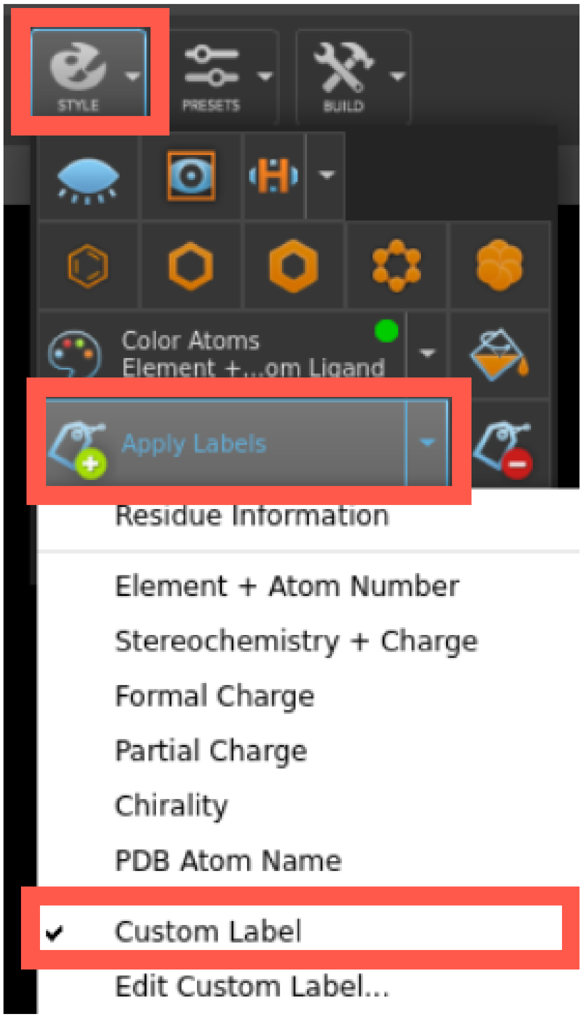

Figure 4-10. Adding element labels.

Figure 4-11. Toggling labels on.

Figure 4-12. Toggling labels off.

17. Go 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

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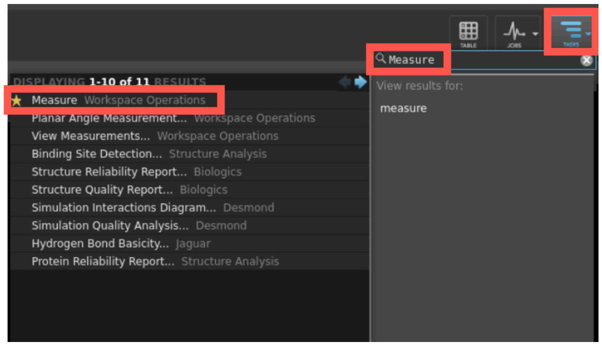
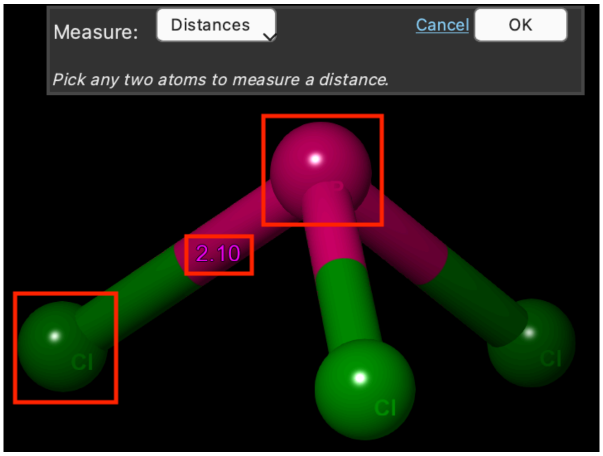


Figure 4-13. Opening the Measure banner

This molecule is not yet optimized. The 3D representation is simply generated from the 2D Sketcher as an approximate starting point. Let's measure the Cl–P bond distance and the Cl–P–Cl angle to assess the starting point:

18. Go to **Tasks > Measure** (or click Measure in the Favorites toolbar)
    - A banner appears at the top of the workspace for defining measurements



Pick any two atoms to measure a distance.

Figure 4-14. Measuring the Cl–P distance.

19. With **Distances** selected for **Measure**, select one Cl atom and the P atom.
    - The Cl–P distance is labeled

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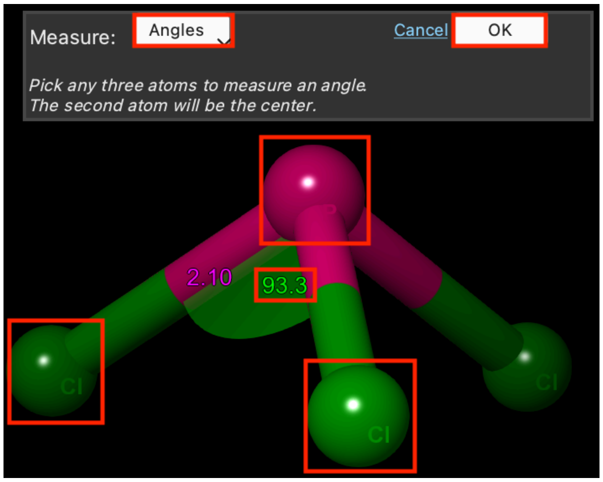

Pick any three atoms to measure an angle.
The second atom will be the center.

Figure 4-15. Measuring the Cl–P–Cl angle.

20. Switch the **Measure** option to **Angles** and select one chlorine, then the phosphorus, and then another chlorine
    - The Cl–P–Cl angle is labeled
21. Feel free to measure the other two Cl–P distances as well as the other Cl–P–Cl angle in PCl_3
22. Click **OK** to close the measurement banner

We can see that the **2D Sketcher** created this 3D starting molecule with the **Cl–P bond lengths equal to 2.10Å** and **Cl–P–Cl bond angles of 93.3º**.

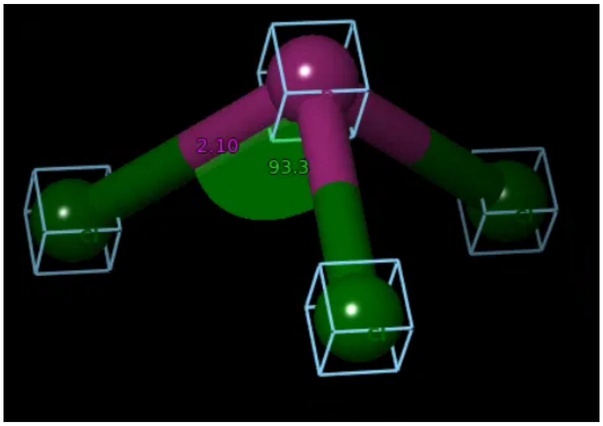

Figure 4-15. Selecting all the atoms in PCl_3.

Part 2. Force Field Minimization

We can improve upon this starting structure by using a force field minimization. The molecule will still not be optimized by quantum mechanics (QM), but it will improve the starting geometry.

1. Select all four atoms in the workspace (there are many approaches to do so: Main Menu, **Select > All**; or, Shift + Click + Drag)
    - You will know all atoms have been selected when each atom is surrounded by a light blue cube.

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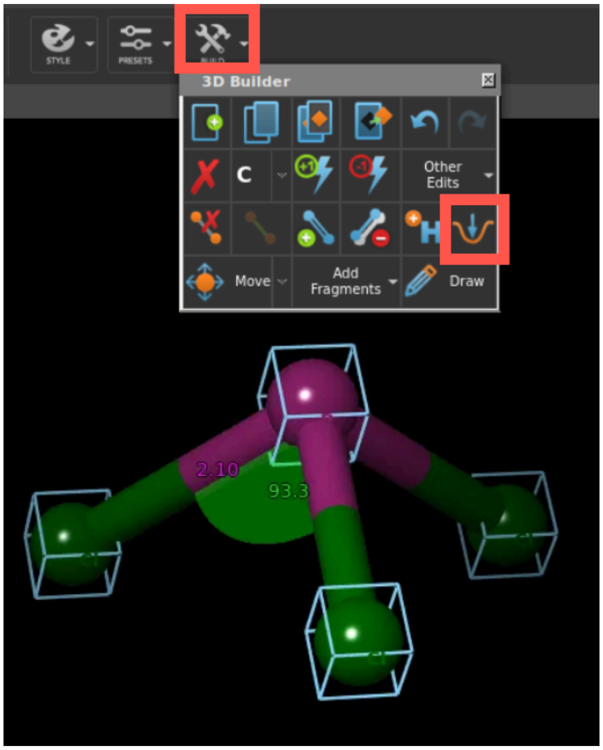

Figure 4-16. Minimizing the geometry of PCl_3.

2. In the **Build** dropdown from the toolbar (**3D Builder panel**), select **Minimize** selected atoms
3. The molecule is minimized, and the parameters adjust slightly

We can now see that the starting molecule has equivalent Cl–P bond lengths still equal to 2.10Å and bond angles of 94.0º. The experimental bond length is 2.07Å and a bond angle of 103º. Thus, the force field minimization improves the structure, but is still somewhat far from being experimentally accurate.

Note: Force fields are usually good at generating structures of molecules with common functional groups and elements. When it comes to more exotic atomic arrangements and less frequent elements (such as transition metals) or simply large molecules, force fields can yield structures with inaccurate or even unphysical geometries, and in those cases, quantum mechanical geometry optimizations become absolutely indispensable.

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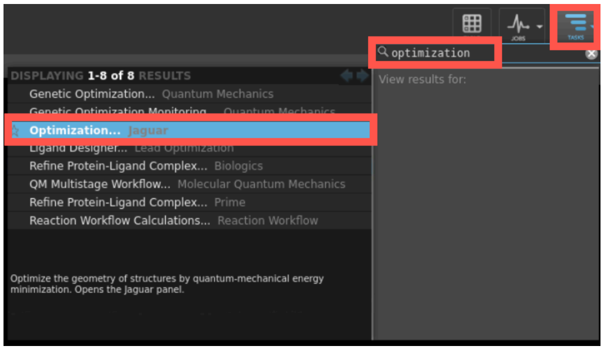
Part 3. Optimize the Geometry using Quantum Mechanic DFT

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

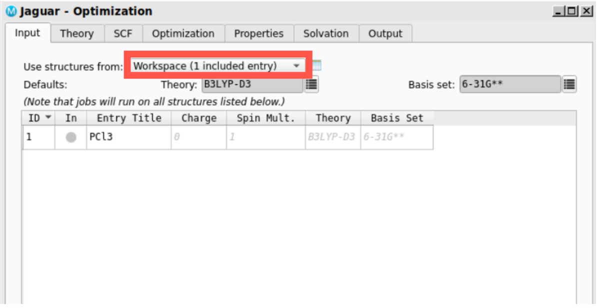
1. Go to **Tasks > Optimization** using Jaguar
    - The Jaguar Optimization panel opens



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

Figure 4-15. Opening up Jaguar from the Tasks bar.

2. Use structures from **Workspace (1 selected entry)**



Use structures from: Workspace (1 included entry)
Defaults: Theory: B3LYP-D3 Basis set: 6-31G**
(Note that jobs will run on all structures listed below.)

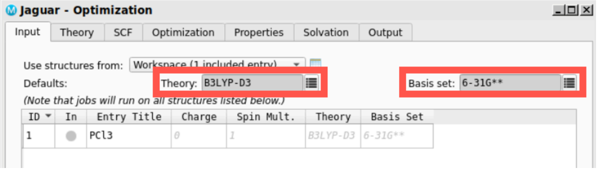
ID	In	Entry Title	Charge	Spin Mult.	Theory	Basis Set
1	●	PCl3	0	1	B3LYP-D3	6-31G**

Figure 4-16. Setting the Jaguar Optimization panel to optimization.

Note: We are optimizing one molecule, PCl_3. By selecting many molecules in the entry list, we can optimize as many molecules as we would like concurrently with the same Quantum Mechanics (QM) settings.

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

3. For Theory, select **B3LYP-D3**
4. For Basis set, select **6-31G****



Use structures from: Workspace (1 included entry)
Defaults: Theory: B3LYP-D3 Basis set: 6-31G**
(Note that jobs will run on all structures listed below.)

ID	In	Entry Title	Charge	Spin Mult.	Theory	Basis Set
1	●	PCl3	0	1	B3LYP-D3	6-31G**

Figure 4-17. Setting the QM parameters for optimization.

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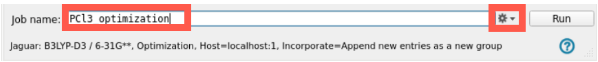
A few additional comments about preparing for an optimization calculation:

- 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, PCl_3 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 and learn more about using the QM Multistage Workflow panel in the Introduction to Multistage Quantum Mechanical Workflows tutorial



Job name: PCl3 optimization

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

Figure 4-18. Naming the job.

5. Change the *Job name* to **PCl3_optimization**

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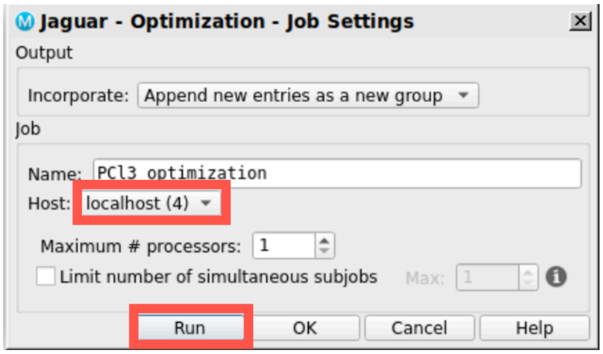


Jaguar - Optimization - Job Settings

Output

Incorporate: Append new entries as a new group

Job

Name: PCl3_optimization

Host: localhost (4)

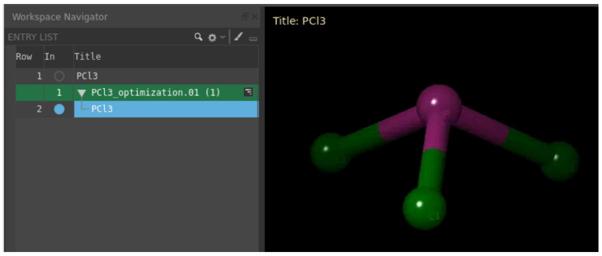
Maximum # processors: 1

☐ Limit number of simultaneous subjobs Max: 1

Figure 4-19. Adjusting the job settings.

6. Adjust the job settings (⚙ ▾)
    - This job requires 1 CPU host and should complete in under 1 minute
7. Click **Run**

Note: It is advised to also add in a Vibrational frequencies calculation (from the Properties tab). This involves a bit more computational expense, but is a useful way to be sure that your output is a minimum (as opposed to a maximum) on the PES. For more detail, see the Locating Transition States: Part 1 tutorial.



Row	In	Title
1	○	PCl3
1		▼ PCl3_optimization.01 (1)
2	●	PCl3

Title: PCl3

Figure 4-20. The output molecule of PCl3.

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

8. A new entry group is added to the entry list titled PCl3_optimization.01 (1). Select and include the molecule titled PCl3 in this sub-group. This is your optimized structure
9. Repeat the measurement steps from above, and measure the P–Cl bond distance and Cl–P–Cl bond angle.

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Now that we have an optimized geometry of PCl_3 that we calculated on Maestro, let's compare our original Lewis-dot structure to the optimized geometry. Since electrons repel one another, the lone pair of electrons on phosphorus push all three chlorine atoms downward to form a trigonal pyramidal geometry. This is why the Cl–P–Cl bond angle was calculated to be 101.1° as opposed to having a 90° angle which the Lewis structure suggests. A simple geometry optimization helps visualize a molecule's true three-dimensional geometry that is otherwise difficult to see just on a piece of paper. Notice that each Cl–P bond is drawn differently in the trigonal pyramidal geometry. One Cl–P bond is drawn on an in-plane bond, another is drawn on a wedged bond which means the Cl atom is going towards you, and another is drawn on a dashed bond which means the Cl atom is going away from you. Drawing bonds with wedges and dashes helps picture the 3-D geometry of the molecule.

Pause & Think #1: Take a screenshot of your optimized structure of PCl_3 including atom labels and any important bond distances or angles. Choose the ball-and-stick representation styling tool.

Original Lewis-Dot Structure of PCl_3	***Trigonal Pyramidal Geometry of PCl_3***	***Optimized Geometry of PCl_3 using DFT***

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Pause & Think #2. Analyze the structure of dichlorodifluoromethane, or CCl_2F_2 by 1) drawing the Lewis structure, 2) performing a geometry optimization using Maestro, and 3) measuring the bond lengths and bond angles listed below. Use the same DFT method as the last example (B3LYP-D3/6-31G**).

Lewis-Dot Structure of CCl_2F_2	**Optimized Geometry of CCl_2F_2 using DFT**	**Bond Measurements from Optimized Geometry**
		● C–F length: ● C–Cl length: ● F–C–F angle: ● Cl–C–Cl angle: ● Cl–C–F angle:

5. Bond Polarity and Electronegativity

Bond polarity is a measure of how equally or unequally the electrons in any covalent bond are shared. A **nonpolar covalent bond** is one in which the electrons are shared equally, like in Cl_2, N_2, or H_2. In the case of Cl_2, each atom starts off with seven valence electrons, and each Cl shares one electron with each other forming one covalent bond.

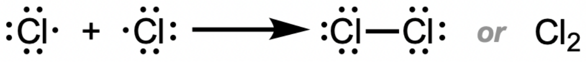

Figure 5-1. Lewis structure of Cl_2

The total number of electrons around each individual atom consists of six nonbonding electrons and two shared, bonding electrons for eight total electrons. This matches the number of valence electrons in the closest noble gas argon (Ar). Since the bonding atoms are identical, Cl_2 contains a nonpolar covalent bond.

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In a **polar covalent bond**, there is an unequal distribution of electrons which is characterized by a partial positive charge on one atom and a partial negative change on the other. The atom that attracts the electrons more strongly acquires the partial negative charge and vice versa. For example, the electrons in the H–Cl bond of a hydrogen chloride atom spend more time near the more electronegative chlorine atom than near the hydrogen atom. Therefore, the chlorine atom carries a partial negative charge while the hydrogen atom has a partial positive charge. We can represent this charge distribution as:

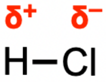
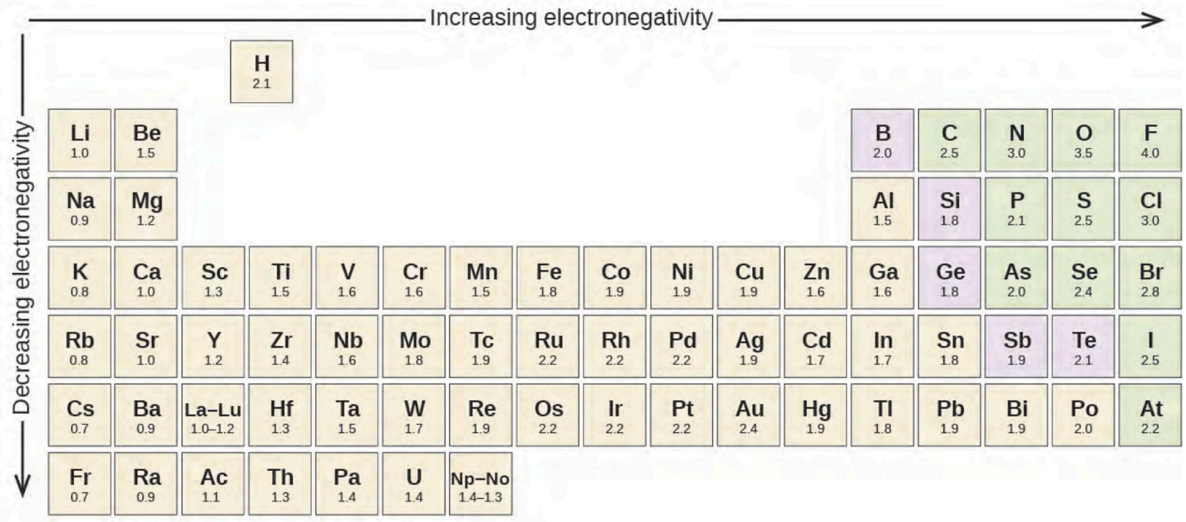


Figure 5-2. Partial charges in H–Cl

The δ^+ (delta plus) and δ^- (delta minus) symbolize the partial positive and negative charges, respectively. In a polar bond, these numbers are less than a full charge of the ions.

Electronegativity is the ability of an atom in a molecule to attract electrons to itself and is used to estimate whether a given bond is nonpolar covalent, polar covalent, or ionic. The greater an atom's electronegativity, the greater its ability to attract electrons to itself. American chemist Linus Pauling developed an electronegativity scale, which is based on thermochemical data shown below.



			H 2.1													
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La–Lu 1.0–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.2
Fr 0.7	Ra 0.9	Ac 1.1	Th 1.3	Pa 1.4	U 1.4	Np–No 1.4–1.3										

Figure 5-3. Linus Pauling's electronegativity scale

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The absolute value of the difference in electronegativity (ΔEN) of two bonded atoms provides a rough approximation of the polarity to be expected in the bond and, thus, the bond type. Note that electronegativity values have no units. When the difference is very small or zero, the bond is nonpolar covalent. When the difference is between 0.4 and 1.8, the bond is polar covalent. When the difference is above 1.8, the bond is ionic. A table summarizing electronegativity differences and bond types is shown below.

Bond Type	Electronegativity Difference
Nonpolar covalent	< 0.4
Polar covalent	0.4 – 1.8
Ionic	> 1.8

Table 5-1. Electronegativity differences based on bond type

Practice #3: Determine the electronegativity differences and bond types of the following fluorine-containing compounds.

	F_2	HF	LiF
ΔEN			
Type of Bond			

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Back to Lesson Contents

<u>Computational Exercise #2:</u> Generating Electrostatic Potential (ESP) Maps on the Molecular Surface

Now we will calculate the electrostatic potential surfaces of F_2, HF, and LiF to help us visually identify a chemical bond type. ESP maps will show the electron-density distribution on the surface of the molecules. This exercise involves four parts:

1) Build the molecules and minimize their geometries
2) Generate surfaces of the molecules
3) Map the electrostatic potentials to the molecular surfaces
4) Label each atom with electrostatic potential values

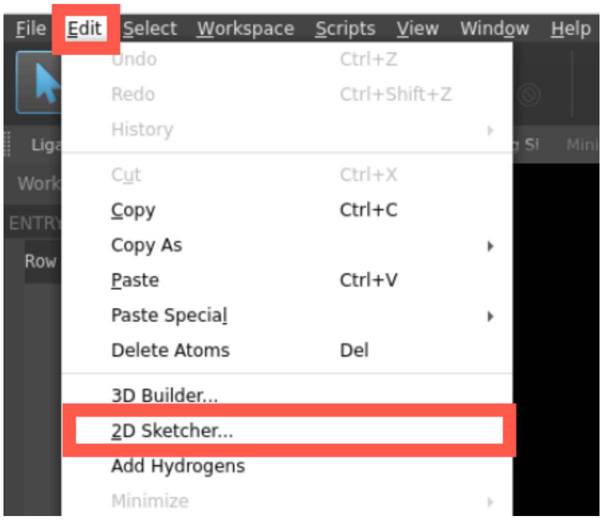

Figure 5-4. Open 2D Sketcher.

Part 1. Build the molecules and minimize their geometries

Before generating any surfaces, build and minimize the structures for F_2, HF, and LiF using the 2D Sketcher tool.

1. Go to Edit > 2D Sketcher. If any existing structures are still in the 2D Sketcher workspace, use the eraser to delete the structure.

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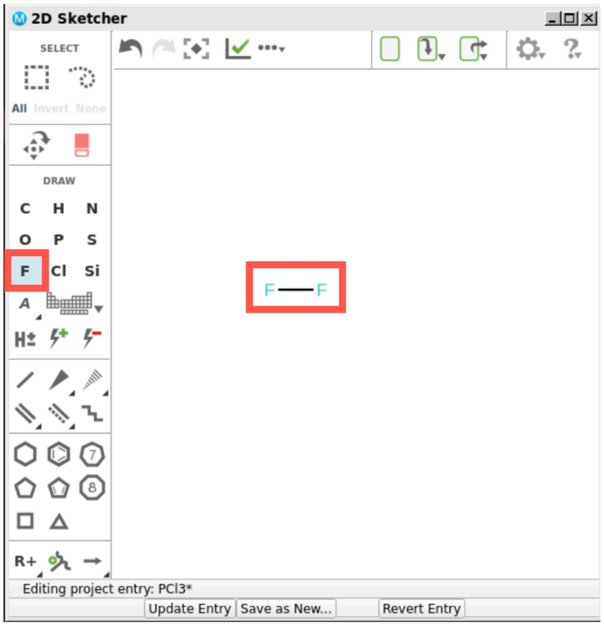
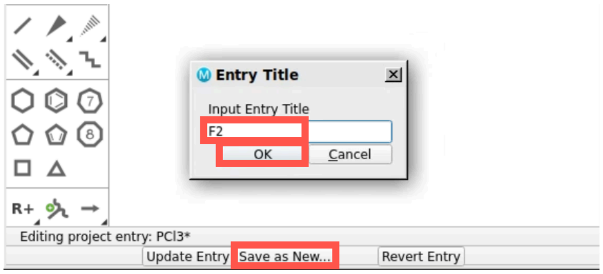


Editing project entry: PCl3*

Figure 5-5. Drawing F_2.

2. **Draw** F_2
    - Go to the selection bar on the left
    - Click the fluorine atom "F" and click in the 2D Workspace to form HF
    - Click "HF" in the workspace to add another fluorine atom



Input Entry Title: F2

Editing project entry: PCl3*

Figure 5-6. Saving F_2.

3. Click on **Save as New** and for **Input Entry Title** write **F2**.
4. Click **OK**.

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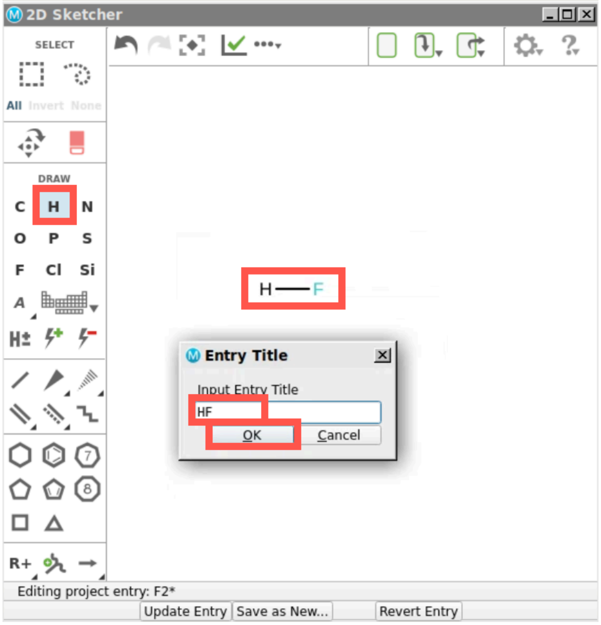
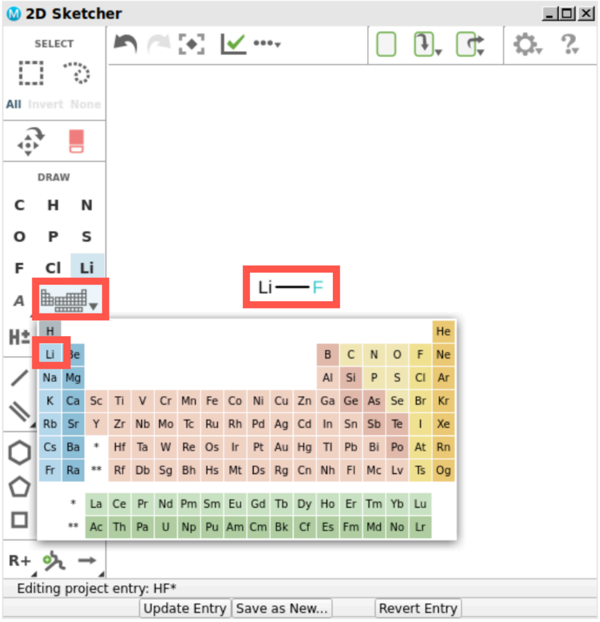


Input Entry Title: HF

Editing project entry: F2*

Figure 5-7. Drawing and saving HF.

5. **Draw** HF
   - Reference the instructions for F_2 in steps 2-4.
   - Replicate the sketch shown in Figure 5-7 as closely as possible.
6. Click on **Save as New** and for *Input Entry Title* write **HF**. Click **OK**.



Editing project entry: HF*

Figure 5-8. Drawing and saving LiF.

7. **Draw** LiF
   - Click the periodic table and select the Lithium atom “Li”
   - Replace the “H” atom with “Li”
8. Click on **Save as New** and for *Input Entry Title* write **LiF**. Click **OK**.

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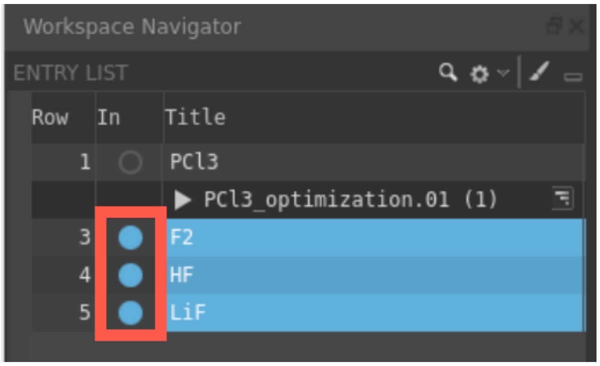

Row	In	Title
1	○	PCl3
		▶ PCl3_optimization.01 (1)
3	●	F2
4	●	HF
5	●	LiF

Figure 5-9. Including all three molecules.

Viewing multiple molecules at the same time can be important for comparing and contrasting them. We will show F_2, HF, and LiF side by side so we can easily see how they differ.

9. Simultaneously include (ctrl + click) all three molecules by clicking each of the circles to the left of each entry name/title

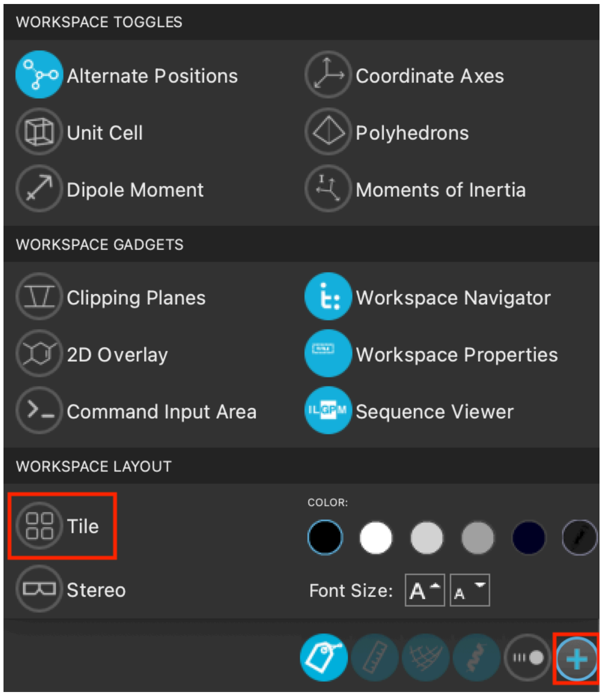

Figure 5-10. Tiling all three molecules.

10. Show **workspace configuration panel** by clicking the **Plus symbol** at the bottom right corner
11. Click **Workspace Layout > Tile**

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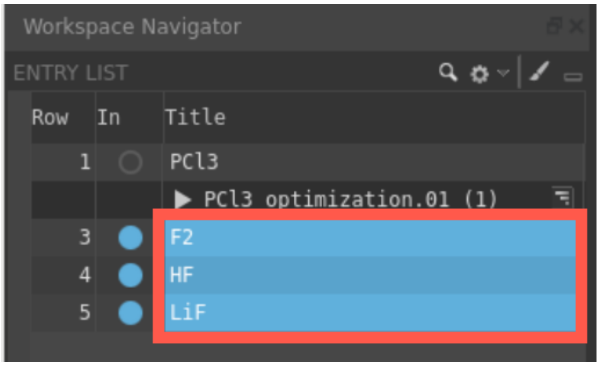

Figure 5-11. Selecting all three entries.

12. Simultaneously select (ctrl + click) all three molecules by choosing all 3 entry names/titles

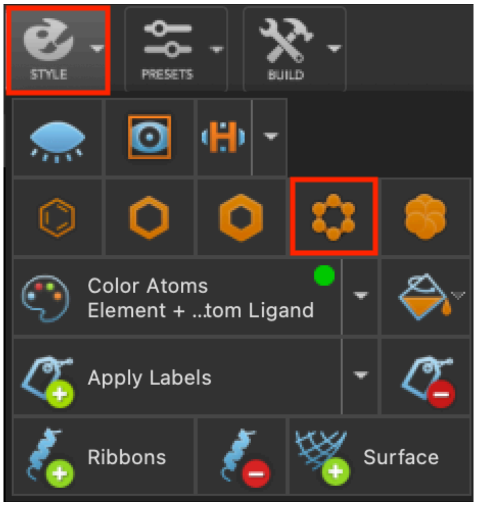

Figure 5-12. Applying ball-and-stick style to all three entries.

13. Change their representations to ball-and-stick by clicking on the **Style** menu and choosing **Apply ball-and-stick representation**
14. Include atom labels if you'd like by clicking **Apply Labels > Custom Label**

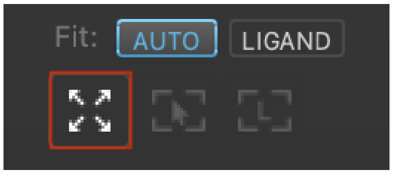

Figure 5-13. Centering the views of all three entries.

15. To center all the molecules within their respective areas, click **Fit view to all visible objects**

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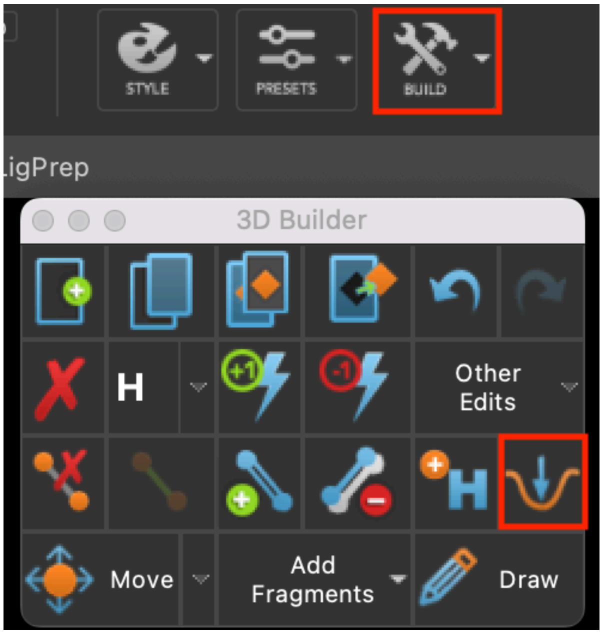
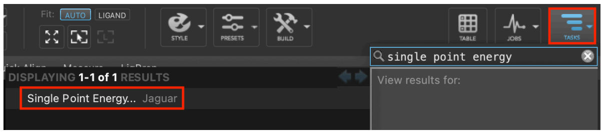


Figure 5-14. Performing force field minimization on all three entries.

16. Select all three molecules in the workspace
17. In the **Build** dropdown from the toolbar (3D Builder panel), select **Minimize** selected atoms
    - The molecule is minimized, and the parameters adjust slightly



single point energy

DISPLAYING 1-1 of 1 RESULTS

Single Point Energy... Jaguar

Figure 5-15. Open the Jaguar - Single Point Energy Panel.

Part 2. Generate surfaces for the molecules

18. Select all three molecules – we will be running the next calculations in parallel (simultaneously)
19. Open the **Jaguar - Single Point Energy** panel from the **Task** button. To do this, click **Browse > Jaguar > Single Point Energy**

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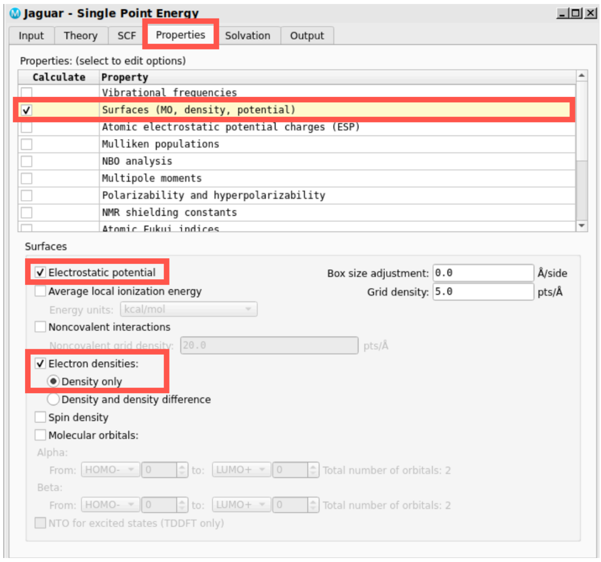


Properties: (select to edit options)

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

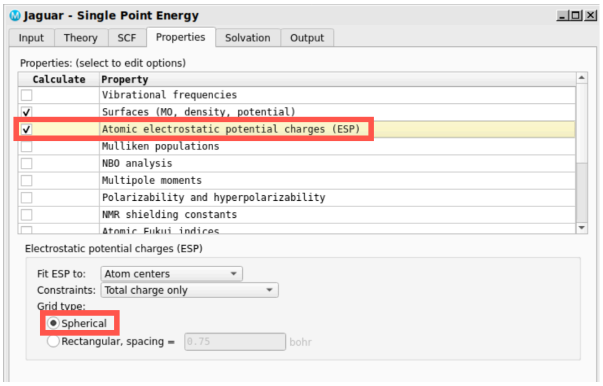
Surfaces

☑ Electrostatic potential
☐ Average local ionization energy
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
☐ NTO for excited states (TDDFT only)

Box size adjustment: 0.0 Å/side
Grid density: 5.0 pts/Å

Figure 5-16. Choosing the surface controls under the Properties tab.

20. Go to the **Properties tab**
21. Select the row for **Surfaces (MO, density, potential)** and click the **check box**
    - The Surfaces controls are displayed at the bottom half of the window
22. In the **Surfaces section**, select **Electrostatic potential** and **Electron densities**, and ensure that no other surface types are selected
23. Ensure that **Density only** is selected under **Electron densities**



Properties: (select to edit options)

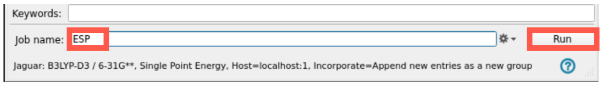
Calculate	Property
☐	Vibrational frequencies
☑	Surfaces (MO, density, potential)
☑	Atomic electrostatic potential charges (ESP)
☐	Mulliken populations
☐	NBO analysis
☐	Multipole moments
☐	Polarizability and hyperpolarizability
☐	NMR shielding constants
☐	Atomic Fukui indices

Electrostatic potential charges (ESP)

Fit ESP to: Atom centers
Constraints: Total charge only
Grid type:
● Spherical
○ Rectangular, spacing = 0.75 bohr

Figure 5-17. Choosing atomic electrostatic potential charges under the Properties tab.

24. Check the box for **Atomic electrostatic potential charges (ESP)** in the **Properties** table
25. Ensure the **Grid type** is **Spherical**



Keywords:
Job name: ESP

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

Figure 5-18. Running the ESP jobs in parallel.

26. Name the job **ESP**
27. Click **Run**
28. When the jobs finish (after 2 minutes or less), the structures are imported and the electron density surfaces may be displayed. The incorporated jobs will be shown in a

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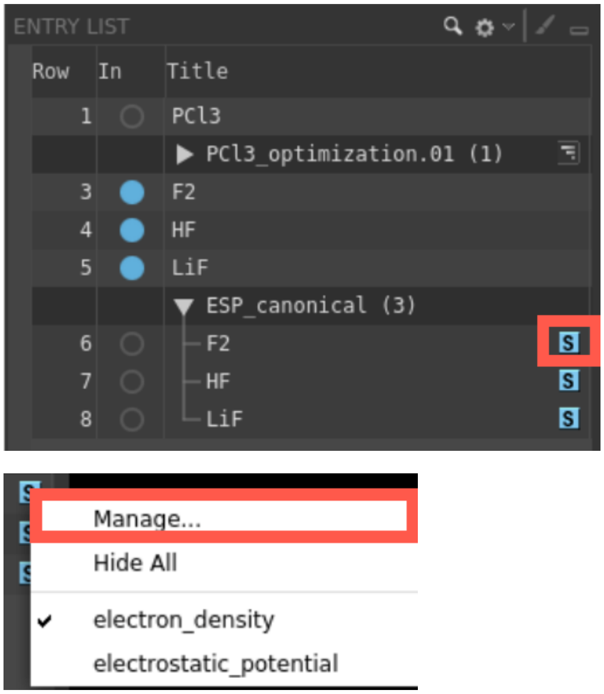
separate Entry Group in the Entry List

Part 3. Map the electrostatic potential to the molecular surfaces

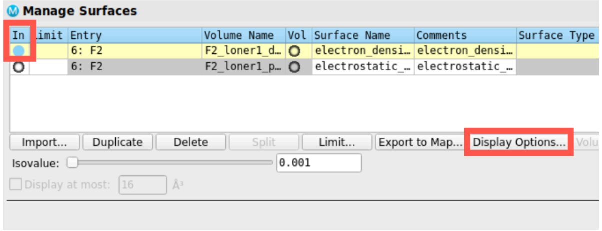
29. Click the **S** button in the **Entry List** for **F2** and choose **Manage**
    - ○ The **Manage Surfaces** panel opens



Row	In	Title
1	○	PCl3
		▶ PCl3_optimization.01 (1)
3	●	F2
4	●	HF
5	●	LiF
		▼ ESP_canonical (3)
6	○	F2 S
7	○	HF S
8	○	LiF S

Figure 5-19. Clicking the S button in the Entry List and choosing Manage.

30. Click the **In** column for the electron density surface to include it in the Workspace
31. Click **Display Options**
    - ○ The Surface Display Options panel opens



Manage Surfaces

In	Limit	Entry	Volume Name	Vol	Surface Name	Comments	Surface Type
●		6: F2	F2_loner1_d…	○	electron_densi…	electron_densi…	
○		6: F2	F2_loner1_p…	○	electrostatic_…	electrostatic_…	

Isovalue: 0.001

☐ Display at most: 16 Å³

Figure 5-20. Choosing settings in the Manage Surfaces panel.

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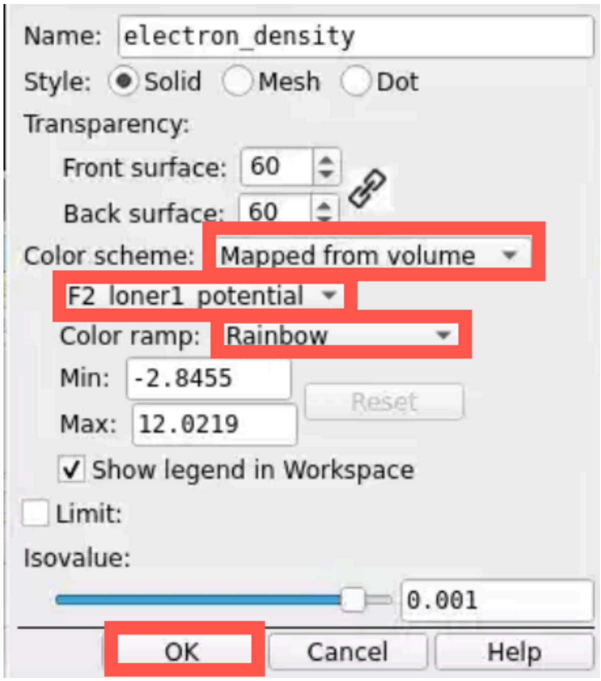

Name: electron_density

Style: ● Solid ○ Mesh ○ Dot

Transparency:

Front surface: 60

Back surface: 60

Color scheme: Mapped from volume

F2_loner1_potential

Color ramp: Rainbow

Min: -2.8455

Max: 12.0219

☑ Show legend in Workspace

☐ Limit:

Isovalue: 0.001

Figure 5-21. Choosing settings in the Surface Display Options panel

32. For **Color scheme**, select **Mapped from volume**
33. Select **F2_loner1_potential** from the **volume data list**
34. From the **Color ramp option menu**, choose **Rainbow**
35. Click **OK**
36. Repeat steps 29-35 for the molecules HF and LiF

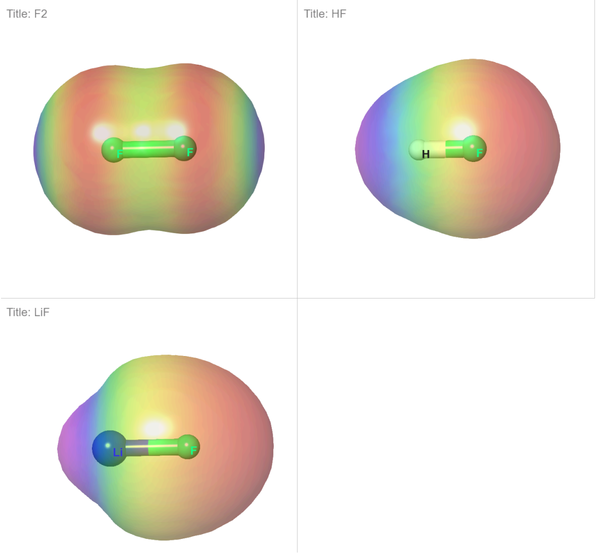

Figure 5-22. Tile all three electrostatic potential surfaces.

37. Once you have displayed all three electrostatic potential surfaces, **Tile** the three molecules so we can compare them
    - Feel free to play around with them and notice any similarities or differences between each molecule

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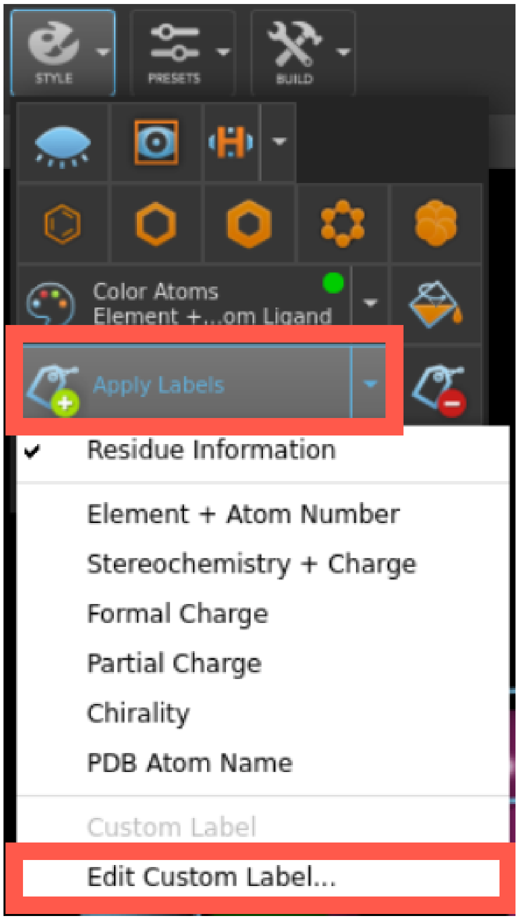

Figure 5-23. Edit custom labels under Style.

Part 4. Label the molecules with electrostatic potential values

38. Select all three molecules in the workspace
39. Click **Style > Apply Labels > Edit Custom Label**
    - The Edit Custom Label dialog box opens

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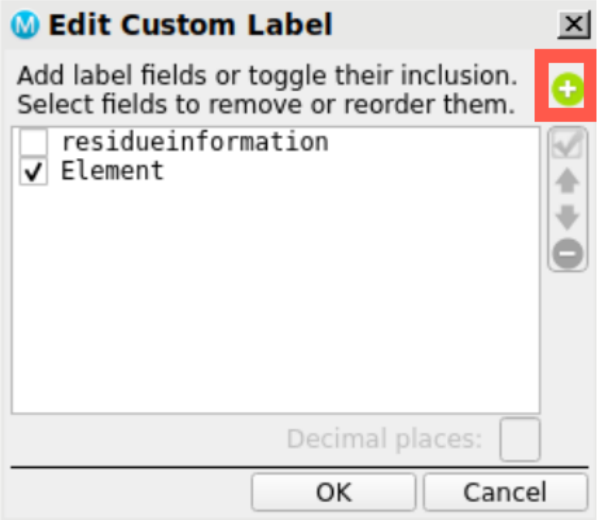

Figure 5-23. Adding label fields.

40. Click **Add** by clicking the **Plus symbol**
    - The Add Label Fields dialog box opens at the Atom Properties tab

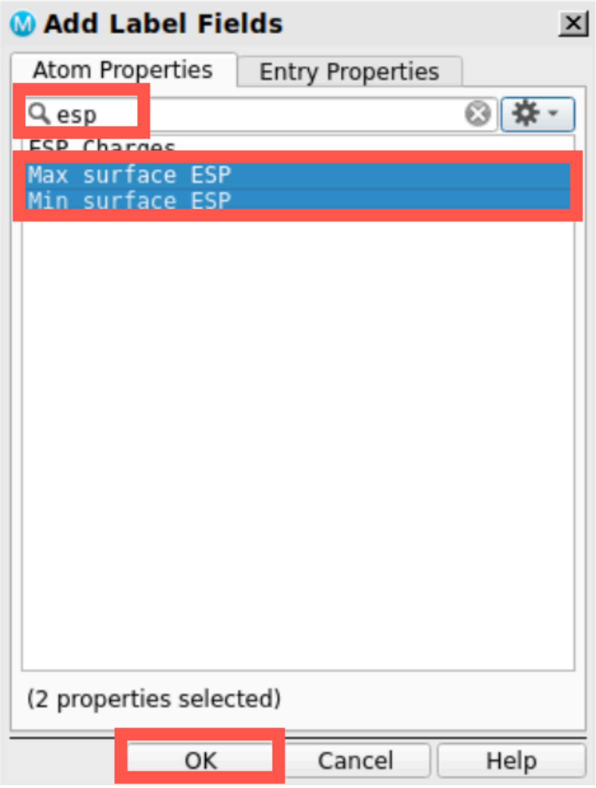

Figure 5-24. Add surface ESP values.

41. Type **ESP** in the search bar and select **Min surface ESP** and **Max surface ESP**
42. Click **OK**
43. **Select** the more electronegative atoms in each molecule:
    - Both F atoms in F_2
    - The F atom in HF
    - The F atom in LiF
44. Go to **Style > Apply Label > Edit Custom Label** and only select **Min surface ESP** in the list and deselect the rest
45. Click **OK**
    - All the electronegative atoms are labeled with their minimum ESP values on the surface, which are negative

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46. **Select** the less electronegative atoms:
    - The H atom in HF
    - The Li atom in LiF
47. Go to **Style > Apply Label > Edit Custom Label** and only select **Max surface ESP** in the list and deselect the rest
48. Click **OK**
    - The H and Li atoms are labeled with their maximum ESP values on the surface, which are positive

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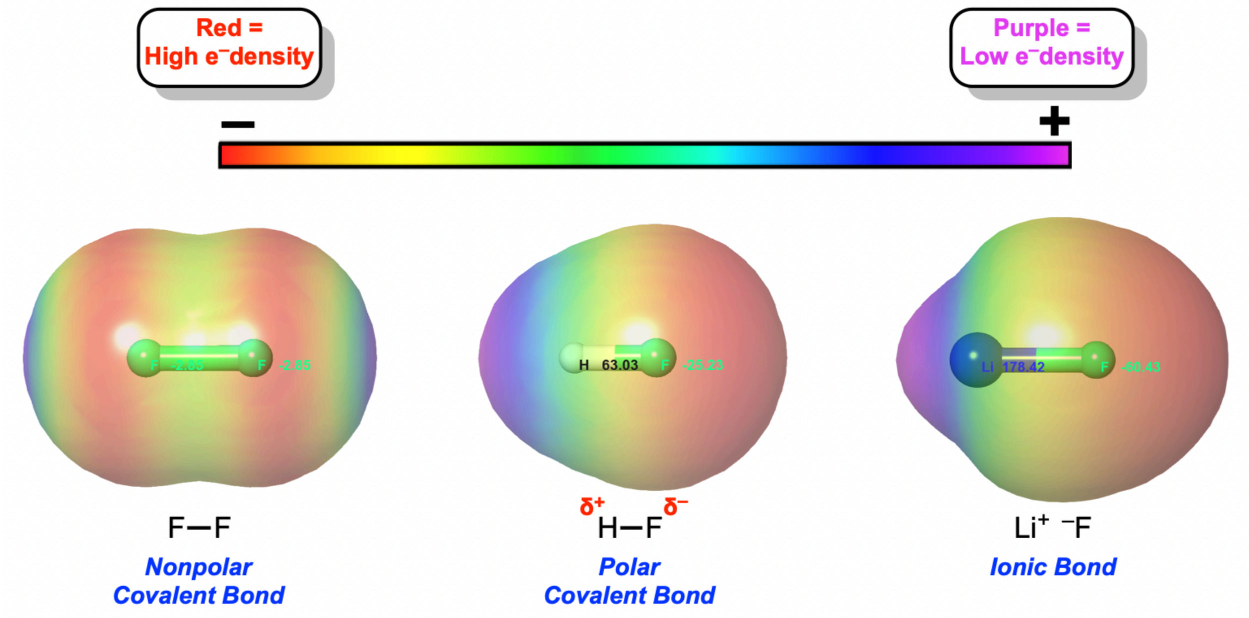
The shift of electron density toward the more electronegative atom in a bond can be seen in each ESP surface. You can see that in F_2 the electron distribution is symmetrical which confirms that the F–F bond is nonpolar covalent. In HF, the electron density is clearly shifted towards fluorine where the more electron dense area is colored red, indicating that the H–F bond is polar covalent due to the larger difference in electronegativity. And in LiF, this shift is even greater as characterized by the more lopsided shape of the overall surface, showing that LiF is an ionic bond.

These examples show that the greater the difference in electronegativity between the two atoms, the more polar their bond is.



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6. Individual Exercises

Determine the electronegativity differences between the following hydrogen halides. Then generate an electrostatic potential surface for each molecule and identify any differences. For the single point calculations, use the following method:

- **Theory:** B3LYP-D3
- **Basis Set:** LACVP++**

Hydrogen Fluoride, H–F	**Hydrogen Chloride, H–Cl**
ΔEN =	**ΔEN =**
ESP Surface:	**ESP Surface:**

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Hydrogen Bromide, H–Br	Hydrogen Iodide, H–I
ΔEN = **ESP Surface:**	**ΔEN =** **ESP Surface:**

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Analysis:

7. Summary, Additional Resources, and References

In this lesson, you learned about chemical bonding and what properties differentiate ionic, nonpolar covalent, and polar covalent bonding. Ionic bonds result from the electrostatic forces that exist between ions of opposite charge. In a polar covalent bond, one of the atoms exerts a greater attraction for the shared electrons than the other. And in a nonpolar covalent bond, the electrons in the bond are shared equally by the two atoms. If we know which atoms are connected to one another, we can draw Lewis structures for molecules and ions.

Using Maestro, a simple geometry optimization using Jaguar can be performed to not only visualize a molecule's structure but also analyze bond lengths and angles. Electrostatic potential surfaces can also be generated to visualize electronegativity trends and analyze chemical bond types.

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For further learning:

- Exploring potential energy surface for chemical reactions: An overview of some practical methods. DOI:10.1002/jcc.10231
- 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

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