

MOLECULAR STRUCTURES AND MOLECULAR GEOMETRIES

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Purpose

The purpose of this laboratory exercise is to draw the structural formulas of molecules and determine their geometries.

Theory

Steps for Drawing Structural Formulas of Covalent Molecules and Polyatomic Ions

Remember that covalent bonds exist between nonmetallic atoms, and that there are different types of substances that contain covalent bonds. Some of these are described below.

- Diatomic elements
- Compounds containing only nonmetals
- Polyatomic ions

Follow these steps to draw structural formulas of molecules and polyatomic ions containing covalent bonds. Sulfur dioxide (SO_2) is used in this example.

1. List the atoms present in the molecule.

- There is one sulfur atom and two oxygen atoms in sulfur dioxide.

S O O

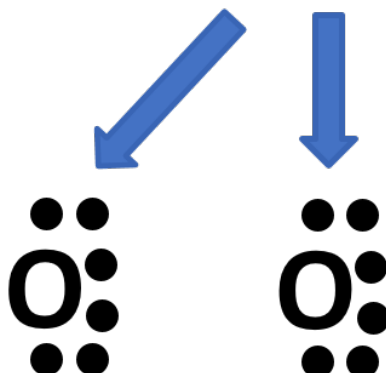
2. Add the total number of valence electrons of all the atoms.

- Every sulfur atom contains 6 valence electrons and every oxygen atom contains 6 valence electrons. So one sulfur atom and two oxygen atoms contains 18 total valence electrons.

**Every sulfur atom has
six valence electrons**



**Every oxygen atom has
six valence electrons**



$$6 + 6 + 6 = 18 = \text{valence electrons}$$

- **Note:** You must take into account the negative or positive charges in this step when determining the structures of polyatomic ions. Add electrons to the total number of valence electrons for polyatomic ions with negative charges, and subtract electrons from the total number of valence electrons for polyatomic ions with positive charges.

For example:

- Add two electrons for a polyatomic ion with a negative two charge.
- Subtract one electron for a polyatomic ion with a positive one charge.

3. Add the electrons required for the octet rule. Remember that you need only 2 electrons for each hydrogen, and 8 (an octet) for all other nonmetallic atoms.

- 8 electrons for each oxygen atom and 8 electrons for the sulfur atom equals 24 electrons needed for the octet rule.

$$8 + 8 + 8 = 24 = \text{electrons needed for octet rule}$$

4. Calculate the number of shared electrons in the molecule.

- (number of octet electrons, calculated in step 3) – (number of valence electrons, calculated in step 2) = number of shared electrons in the molecule

$$24 - 18 = 6 = \text{number of shared electrons in the molecule}$$

5. Determine the most symmetrical arrangement of atoms for molecules with more than two atoms.

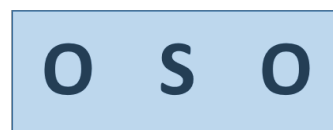
- For many small molecules (molecules with 6 or few atoms) there will be an atom in the middle of the molecule (the central atom), and all the other atoms will be bonded to the central atom.
- Assume that in the SO_2 molecule two atoms are bonded to a central atom.
- Determine the most symmetrical arrangement of the atoms assuming this type of structure.
- Consider the three arrangements of atoms below. In each case there is a central atom. Notice that the structure with the sulfur atom as the central atom is the most symmetrical.



- The oxygen atom is the central atom.
- Not the most symmetrical arrangement



- The oxygen atom is the central atom.
- Not the most symmetrical arrangement

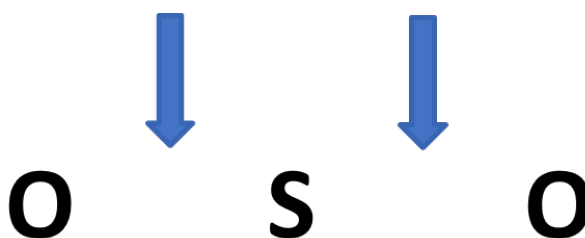


- The sulfur atom is the central atom.
- The most symmetrical arrangement

- Also notice that this molecule must have two bonds. One bond is needed to connect each atom to the central atom.

A bond is needed here

A bond is needed here



6. Divide the number of shared electrons in the bonds.

- There are two bonds in this molecule, and there are 6 shared electrons in the molecule (calculated in step 4).

So the molecule has one single bond and one double bond connecting the three atoms.

- This is the only way to divide 6 shared electrons into two bonds.
- Remember that:
 - One single bond between two atoms has 2 shared electrons
 - One double bond between two atoms has 4 shared electrons
 - One triple bond between two atoms has 6 shared electrons.

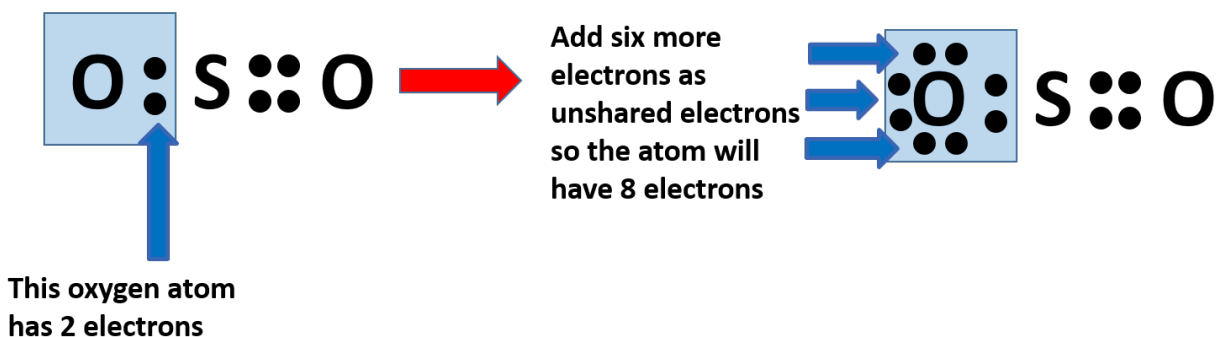
Two shared electrons (one single bond) connecting these two atoms

Four shared electrons (one double bond) connecting these two atoms

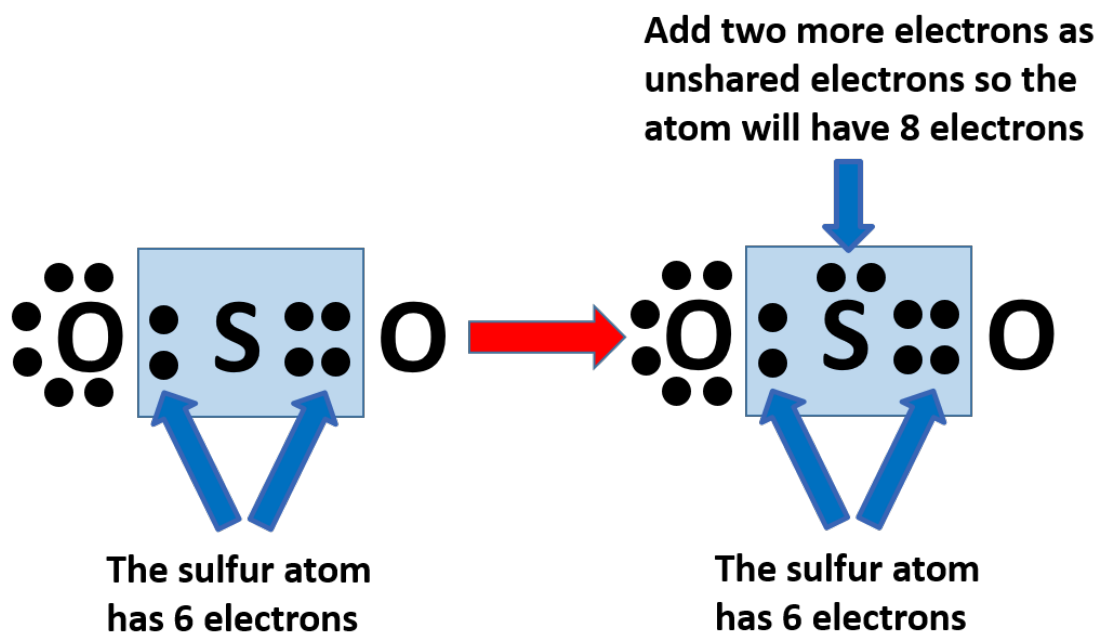


7. Draw the unshared electrons so that all of the atoms have an octet.

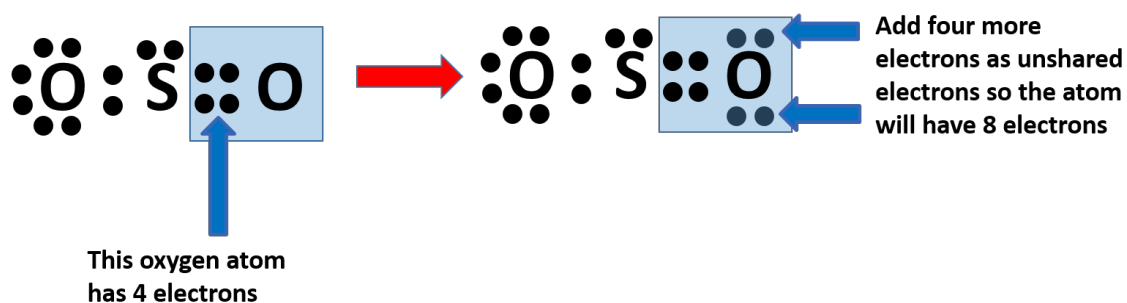
- This oxygen atom has two electrons. Add six more electrons as unshared electrons so the atom will have 8 electrons (an octet).



- The sulfur atom has two electrons. Add six more electrons as unshared electrons so the atom will have 8 electrons (an octet).



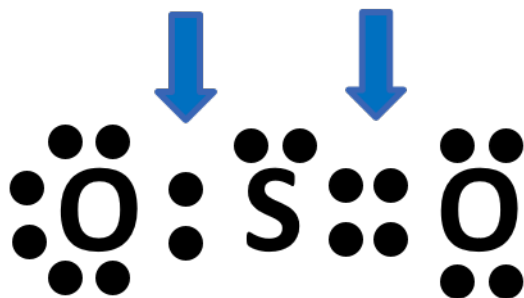
- This oxygen atom has four electrons. Add four more electrons as unshared electrons so the atom will have 8 electrons (an octet).



- The final structure has one single bond and one double bond.

**Two shared electrons
is one single bond**

**Four shared electrons
is one double bond**

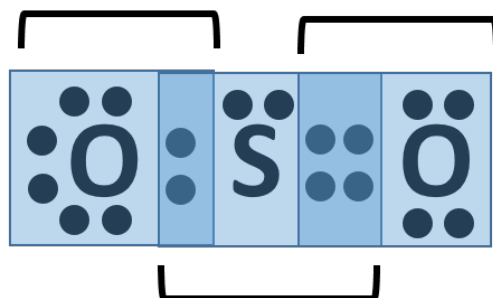


8. Check your answer. Make sure that all of the atoms follow the octet rule.

- All three atoms have an octet which is correct

**This oxygen atom
has 8 electrons. It
has an octet and is
stable.**

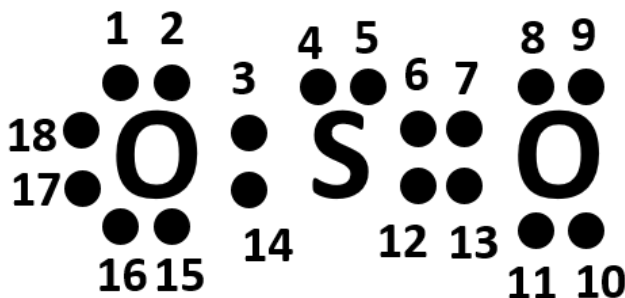
**This oxygen atom
has 8 electrons. It
has an octet and is
stable.**



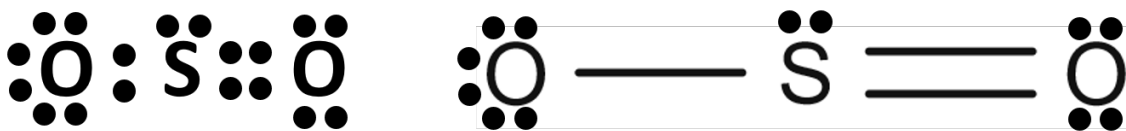
**The sulfur atom
has 8 electrons. It
has an octet and is
stable.**

9. Count the total number of electrons you drew. The number of shared electrons plus the number of unshared electrons must equal the total number of valence electrons that you calculated in step 2.

- The total number of valence electrons calculated in step 2 is 18 electrons. The molecule shows 18 total electrons.



Based on these steps, the correct electron—dot structure and structural formula for SO_2 are below.



Determining the Molecular Geometries of Covalent Molecules and Polyatomic Ions

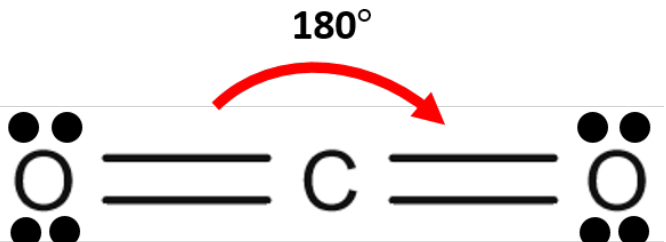
As described above, the structural formulas of molecules and polyatomic ions can be determined by following several steps. The **molecular geometry** or shape of a molecule can be determined once the structural formula is known.

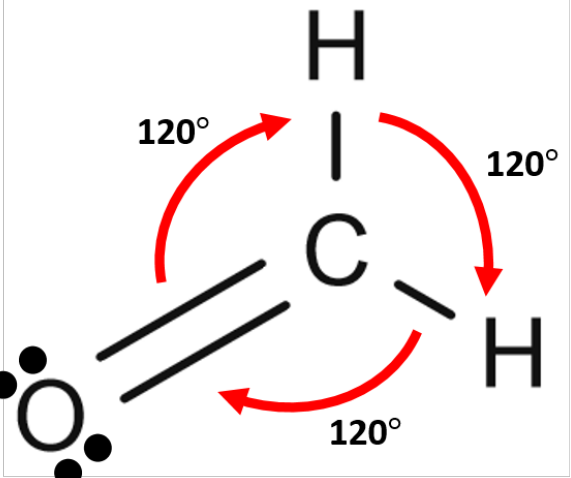
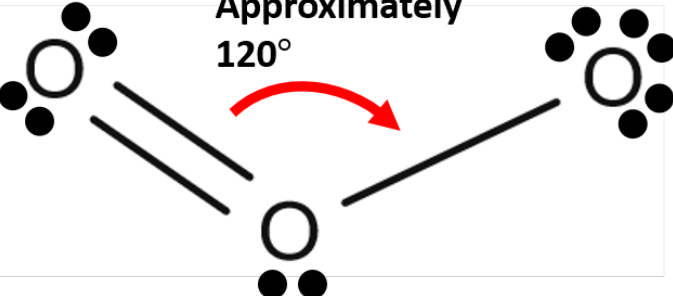
The molecular geometry is the three-dimensional shape of the molecule or ion. The geometry depends on the number of bonds and the number of pairs of unshared electrons connected to the central atom.

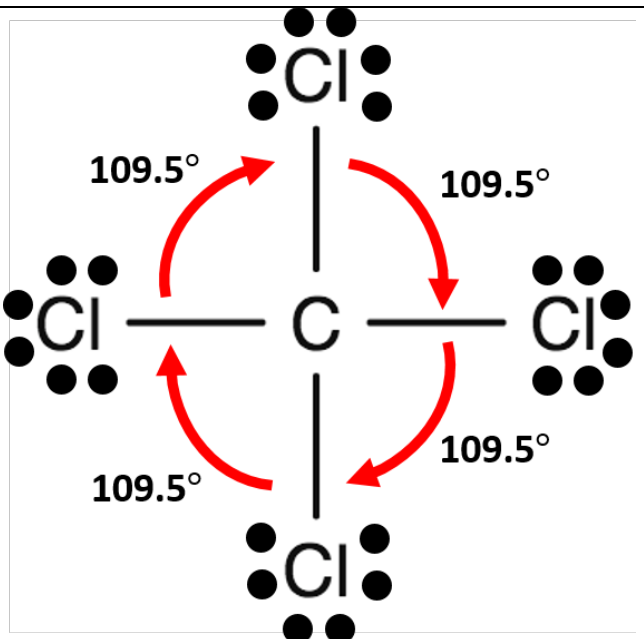
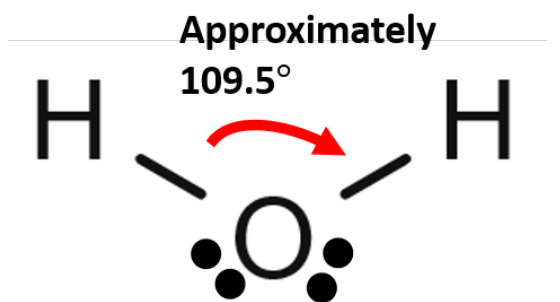
The tables on the following pages show the common molecular geometries of molecules and how these geometries are effected by the number of bonds and pairs of unshared electrons on the central atom.

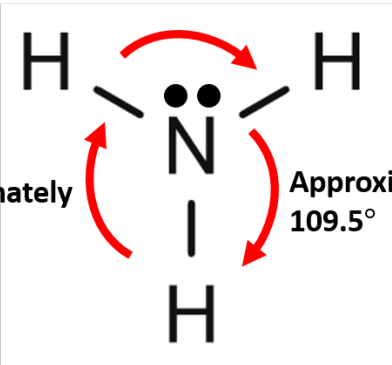
The table below summarizes the common molecular geometries seen in covalent molecules and polyatomic ions. Notice the following.

- Molecules with the same number of electron densities on the central atom (the same total number of bonds and pairs of unshared electrons) have the same or similar bond angles. (See shading in table.)
- All linear and bent molecules have **two bonds** connected to the central atom. Linear molecules have 180° bond angles and bent molecules have bond angles less than 180° .
- All trigonal planar and pyramidal molecules have **three bonds** connected to the central atom. Trigonal planar molecules have 120° bond angles and pyramidal molecules have approximately 109.5° bond angles.
- All tetrahedron molecules have **four bonds** connected to the central atom. Tetrahedron molecules have 109.5° bond angles.

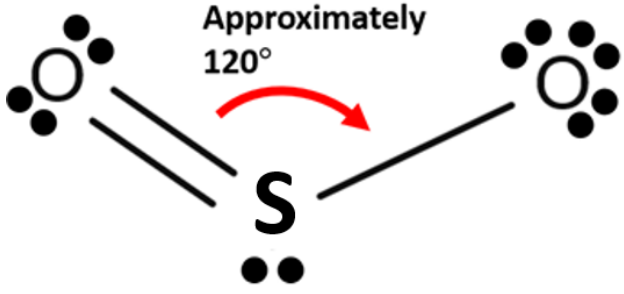
Molecular geometry	Total number of bonds and electron pairs on central atom	Bonds connected to central atom	Pairs of unshared electrons on the central atom	Bond angles	Examples
Linear	2	2	0	180°	

Trigonal planar	3	3	0	120°	
Bent	3	2	1	Approximately 120°	

Tetrahedron	4	4	0	109.5°	
Bent	4	2	2	Approximately 109.5°	

Pyramidal	4	3	1	Approximately 109.5°	Approximately 109.5°  Approximately 109.5°
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The sulfur dioxide molecule has two bonds and two unshared electrons (one pair of electrons) on the central atom. So the sulfur dioxide has a bent shape with a bond angle of approximately 120 degrees.

Molecular geometry	Total number of bonds and electron pairs on central atom	Bonds connected to central atom	Pairs of unshared electrons on the central atom	Bond angles	Sulfur Dioxide
Bent	3	2	1	Approximately 120°	

Name _____

Date _____

MOLECULAR STRUCTURES AND MOLECULAR GEOMETRIES

Procedure, Data Sheet and Questions

A. Determining Structural Formulas

1. Determine the structural formulas of the five molecules and polyatomic ions in the table below using the steps described in the **Theory** section, and answer questions about the structures. Sulfur dioxide is in the table as an example.

Formula	Central atom	Number of single bonds connected to the central atom	Number of double bonds connected to the central atom	Number of triple bonds connected to the central atom	Number of pairs of unshared electrons on the central atom
SO ₂	S	1	1	0	1
CS ₂	C	0	2	0	2
NF ₃	N	3	0	0	1
H ₂ S	S	2	0	0	2
NO ₂ ⁻	N	1	1	0	1
SO ₃ ²⁻	S	2	1	0	1

B. Determining Molecular Geometries

1. Determine the molecular geometries of the five molecules and polyatomic ions in the table below using the information in the **Theory** section and the information you completed on the previous page. Sulfur dioxide is in the table as an example.

Formula	Molecular geometry	Total number of bonds and electron pairs on central atom	Bonds connected to central atom	Pairs of unshared electrons on the central atom	Bond angles
SO₂	Bent	3	2	1	Approximately 120°
CS₂	Linear	4	2	2	180 °
NF₃	Pyramidal	3	3	1	109.5 °
H₂S	Bent	2	2	2	109.5 °
NO₂⁻	Bent	3	2	1	120 °
SO₃²⁻	Trigonal Pyramidal	4	3	1	109.5 °