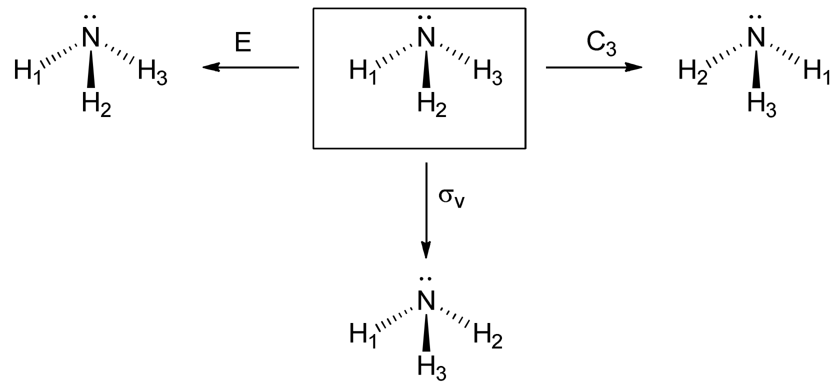
Model 1: Ammonia

In groups, consider the three dimensional ammonia molecule in the box below. You may find it useful to use a model kit to build one or more molecules. (Hint: It will be easier to see changes in position of atoms if all H atoms are not the same color.) For each question you must agree on the answer before moving to the next question.



Critical Thinking Questions

1. How does the ammonia molecule in the box change when 'E' is applied?

   Students should recognize that the molecule remains the same.

2. How does the ammonia molecule in the box change when 'C_3' is applied? (Hint: What does the 3 tell us?)

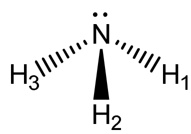
   Students should notice that the molecule is rotated or turned.

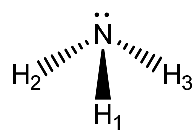
3. How does the ammonia molecule in the box change when 'σ_v' is applied?

   Students should recognize that H_2 and H_3 switch spots. Some students might mention that there is a reflection through the N-H_1 bond

4. When a 'σ_v' is applied to the molecule, the structure of the molecule before 'σ_v' is identical to the structure of the molecule after 'σ_v'. Draw the other two possible results when 'σ_v' is applied to the ammonia molecule in the box. The 'σ_v' is also called a 'mirror plane'. How many such mirror planes are there in ammonia? (Hint: Use a model kit to help you see changes in the positions of atoms.)

   The goal of this question is to get students to realize that there is more than one 'σ_v'. Also, students should realize that atoms don't come with subscripts. If they use the same color atoms from their model kits for each hydrogen then the molecules should look identical.

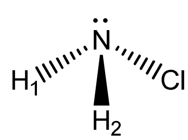




5. Draw the Lewis structure for NH_2Cl and label each hydrogen atom with a different subscript similar to the ammonia molecule above. (Hint: Some starting orientations might make it easier to see other symmetry operations than others.)

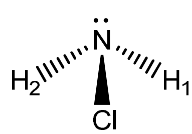
   Students may draw different orientations of the NH_2Cl molecule. The next few questions are going to be dependent on the initial structure drawn. ***If several groups seem to be struggling with this question, it might be helpful to have one student from each group (reporter) draw their structures on the board and then have a large group discussion.***

   a. If an 'E' can be applied, draw the NH_2Cl molecule.

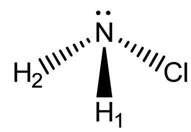


   b. If a 'C_3' can be applied, draw the NH_2Cl molecule.

   Students should realize that this isn't possible based on the description from question 4, however, if students draw a structure here they will be asked in question 9 to re-examine their answer to this question after symmetry operations and symmetry elements are introduced and defined. An example structure that students may draw would be:



c. If a 'σ_v' can be applied, draw the NH_2Cl molecule.



Information

All molecules can be described in terms of symmetry. Here are several different statements to describe what is meant by 'symmetry operation'.

A symmetry operation is a movement of a body such that after the movement has been carried out every point of the body looks like it is in its original position.

If you close your eyes when the symmetry operation is performed, and, if you cannot tell that the operation has occurred after you open your eyes, then it was a valid symmetry operation.

"A symmetry element is a geometrical entity such as a line, plane or point that can be used to carry out a symmetry operation." (Cotton, 1971).

In order for the operation to be considered symmetrical, the position and orientation of the atoms relative to one another within the molecule must be the same after the operation as it was before the operation.

Critical Thinking Questions

6. Identity Symmetry Operation:

   a. Define the identity symmetry operation, 'E'. (Everyone in the group must agree.)

   Students should mention that the structure orientation doesn't change.

   b. Will all molecules have the identity symmetry operation, 'E'? Explain.

   Yes, the identity symmetry operation should apply to all molecules since the structure orientation doesn't change when E is applied.

7. Rotation symmetry operation:

   a. Define the rotation symmetry operation, 'C_3'.

   Students should mention that the structure is rotated 1/3 the way or 120 degrees.

   b. Will all molecules have the rotation symmetry operation, 'C_3'? Explain.

   No, not all molecules will have the possibility to rotate the structure 120 degrees and have the orientation be the same.

   c. What does the 3 in 'C_3' tell us about the rotation symmetry operation?

   The molecule can be rotated 3 times in order to rotate 360 degrees.

8. Reflection symmetry operation:

   a. Define the reflection symmetry operation, 'σ_v'.

   Students should mention that the molecule is reflected through a plane. Some students might recognize that it is a reflection over a bond.

   b. Will all the molecules have the reflection symmetry operation, 'σ_v'? Explain.

   No, *not all molecules will have the reflection symmetry operation. In order for a reflection operation there has to be a plane that the molecule is reflected through.*

9. Given your definition of a C_3 symmetry operation, would you answer question 5b any differently now? If yes, how?

   If students said that a C_3 was not possible they should answer this question: no.

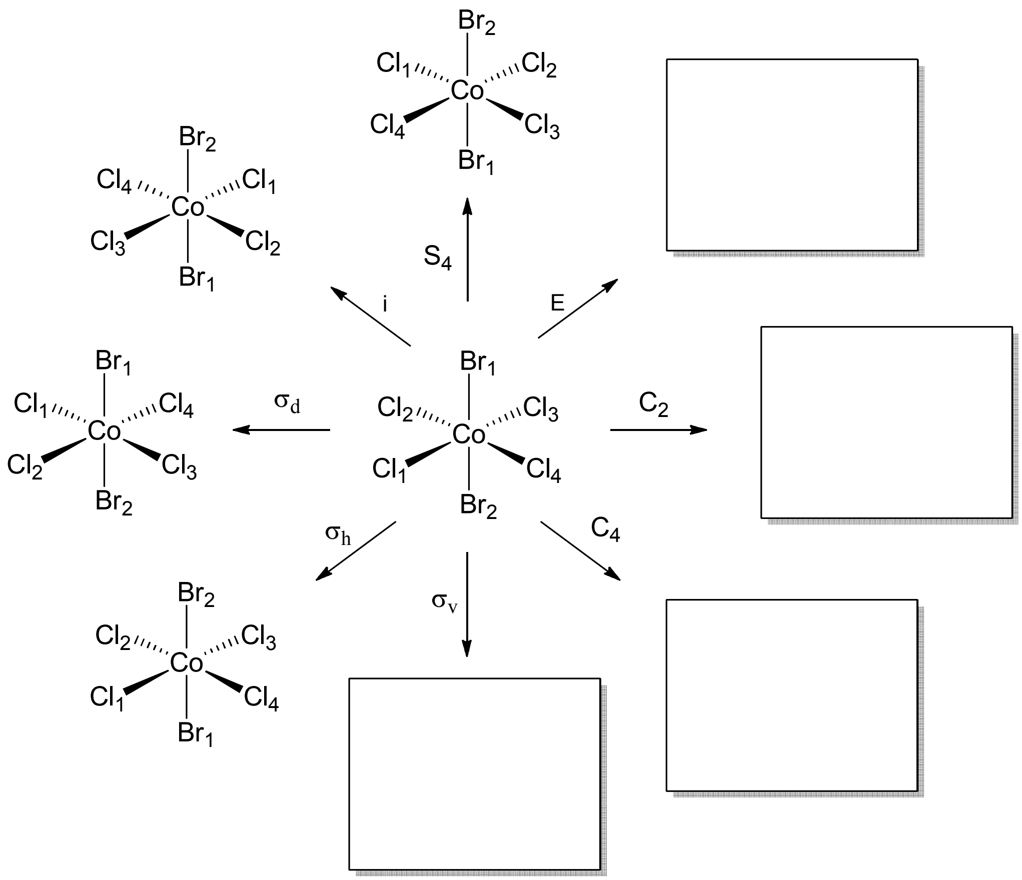
   If students said that a C_3 was possible, then they should answer this question: yes, now realizing that a C_3 is not possible because the atoms are in different positions.

References

Cotton, Albert F. *Chemical Applications of Group Theory*, 2nd Ed. John Wiley & Sons: New York, 1971.

Model 2: *trans*-dibromotetrachlorocobaltate(3-)

Consider the three-dimensional structure for *trans*-dibromotetrachlorocobaltate(3-).



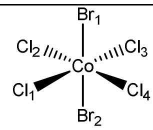
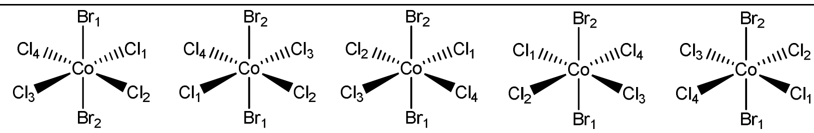
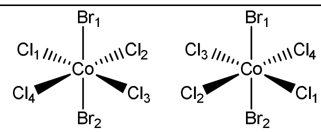
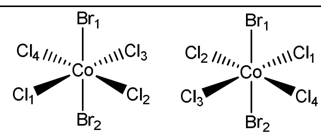
Critical Thinking Questions

10. Fill in the boxes in the model as a group, and then draw the structures on the board.

Students only need to draw one molecule in each box. This is a good point to have each group draw their molecules on the board. The groups should realize that there is more than one possible structure for C_2, C_4, and σ_v. A complete list of possible structures is provided in the table below. This is also a good place to point out that a rotation goes clockwise around the axis of rotation.

Possible structures for each box:

Symmetry Operations	*Possible structures* ***(Students are asked to draw only one structure for***

	each operation)
E	
C_2	
C_4	
σ_v	 Some students might draw the structure with the plane of reflection going between the Cl atoms (σ_d). This will be addressed in question 17 when the student needs to determine the differences between σ_v and σ_d.

11. Rotation symmetry operations:

    a. How does a 'C_2' differ from a 'C_4'?

    Students should realize that a C_2 is a 180 degree rotation (360/2) and a C_4 is a 90 degree rotation (360/4). Therefore, two C_4's done in succession are equivalent to one C_2 operation which will be explored again in question 21.

    b. What does a 'C_n' symmetry operation involve?

    Students should realize that the rotation degree is 360 degrees/n.

    c. A principle rotation axis is the rotation axis with the highest n value.

        i. What is the principle rotation axis for Model 1?

C_3

ii. What is the principle rotation axis for Model 2?

C_4

12. How does the starting orientation change when 'σ_h' is applied?

Students should notice that only the Br groups move. Some might say it is a reflection through the plane containing the Co and Cl atoms.

13. Reflection symmetry operation, 'σ_h':

a. Define the reflection symmetry operation, 'σ_h'.

Students should notice that only the Br groups move. Some might say it is a reflection through the plane containing the Co and Cl atoms.

b. Will all molecules have the 'σ_h' reflection symmetry operation? Explain.

No, because a 'σ_h' is a reflection through a plane that is horizontal (perpendicular) to the C_4 rotation axis which is the highest principal rotation axis and not all molecules will have this plane of reflection.

14. How does the central molecule change when 'σ_d' is applied?

Students should notice that there is a reflection through a plane containing the Co and Br atoms and passing between the Cl_3 and Cl_4 atoms.

15. Reflection symmetry operation, 'σ_d':

a. Define the reflection symmetry operation, 'σ_d' .

Students should mention that it is a reflection through a plane that contains the C_4 rotation which is the highest principal rotation axis and contains no other atoms in the molecule other than the atoms that fall on the rotation axis.

b. Will all molecules have the 'σ_d' reflection symmetry operation? Explain.

No, because it is a reflection through a plane that contains the C_4 rotation which is the highest principal rotation axis and contains no other atoms in the molecule other than *the atoms that fall on the rotation axis. Not all molecules will have a plane of reflection that includes the principle rotation axis but not other atoms beyond the ones in the rotation axis.*

16. What is the difference between a 'σ_v' and a 'σ_d'?

    The 'σ_v' reflection plane contains two Cl atoms while the 'σ_d' reflection plane doesn't contain any Cl atoms.

17. How does the central molecule change when 'i' is applied?

    Each atom changes place with the atom directly across. All the atoms except for the central atom change position.

18. Inversion symmetry operation, 'i':

    a. Define the inversion symmetry operation, 'i'.

    All atoms are passed through a central point within the molecule which is called the point of inversion.

    b. Will all molecules have the inversion symmetry operation, 'i'? Explain.

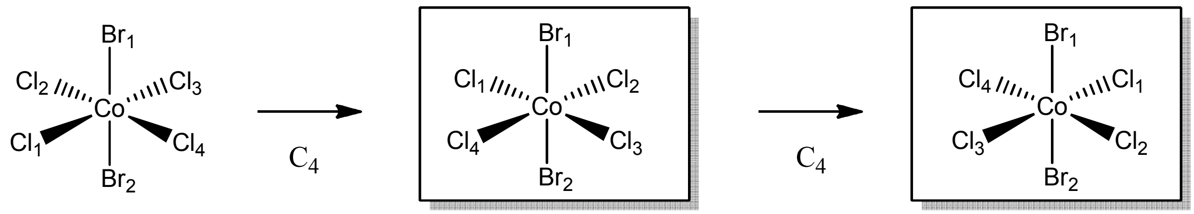
    No, not all atoms have a central spot that will allow all the atoms to switch places with the atoms directly across. ***Some students will find it really hard to picture what is going on in the inversion symmetry operation. An easy way to help students get through this is to prompt students to imagine a point (x,y,z) and move it to point (-x,-y, -z).***

19. How does the starting orientation change when 'S_4' is applied?

    The Br atoms exchange places and the Cl atoms all rotate 90 degrees clockwise.

20. Some symmetry operations are equivalent to a combination of symmetry operations.

    a. Fill in the boxes below. How can you get from the initial structure orientation to the final structure orientation using only one kind of symmetry operation?



Students should realize that a C_2 will give them the same structure as two C_4 symmetry operations done consecutively.

b. Looking back at Model 1 and Model 2, which two symmetry operations can lead to the improper rotation symmetry operation, 'S_4'?

Students should notice that if C_4 and σ_h are combined you arrive at the S_4 structure. ***This question might take students a little longer than the other questions to realize which two symmetry operations need to be combined. If students are struggling too much, the instructor could have students look back at question 20 and see if they can notice that there is a rotation and something else present.***

21. Improper rotation symmetry operation, 'S_n':

a. Define the improper rotation symmetry operation, 'S_n'.

An improper rotation symmetry operation is a rotation about any Cn axis, followed by a reflection through the plane that is perpendicular to that axis of rotation.

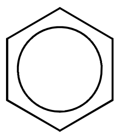
b. Will all molecules have the improper rotation symmetry operation, 'S_n'? Explain.

No, not all molecules have a rotation possible and of the ones that do have a rotation, not all molecules have a reflection that is perpendicular to the axis of rotation.

Exercise Questions

1. Find the principle rotation axis for the following molecules. Label it as C_n by specifying the value of n.

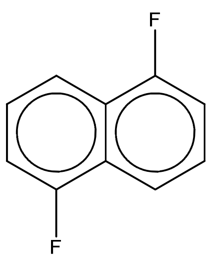
    a. Benzene

    n=6

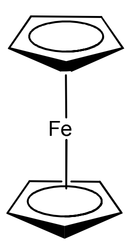
    Students should treat all bonds in benzene as equivalent so this molecule has a C_6

    b. 1,5-difluoronaphthalene

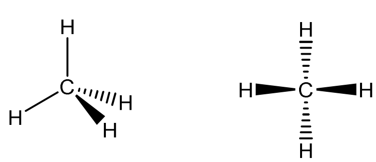
    n=2

    c. Eclipsed ferrocene

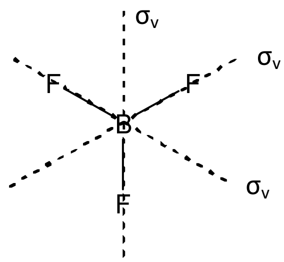
    n=5

    d. Methane, CH_4 *n=3*

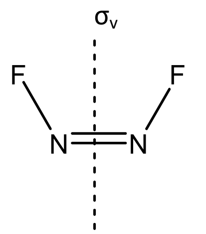
    

    Students need to draw their structure and analyze the structure. N=2 is also possible but not the highest order rotation axis.

2. Determine how many planes of reflection are in each of the following molecules. Show the location and label each reflection plane.

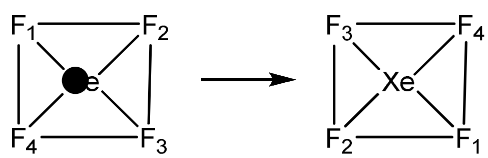
a. 

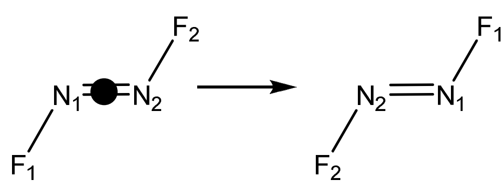
A σ_h is in the plane of the paper

b. 

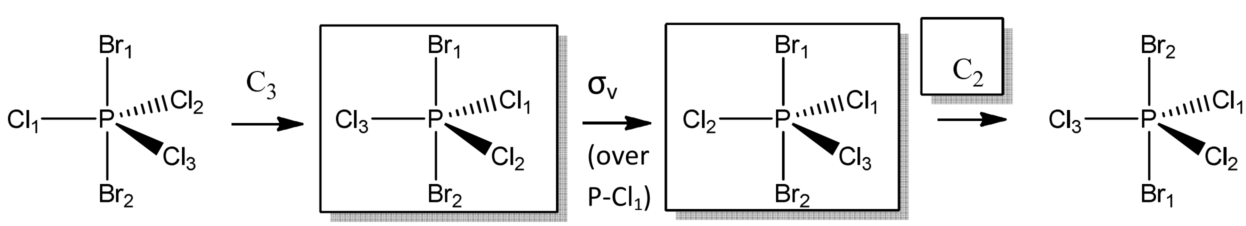
Another σ_v is in the plane of the paper

3. Show the center of inversion on the following molecules with a dot. Draw the structure after the inversion takes place.

a. 

b. 

4. Fill in the following boxes.



The C_2 axis is along the P-Cl_1 bond.