MoleCVUE Activity *level* - Inorganic Chem

Determining symmetry elements and point groups from molecular structures

Introduction and Overview

You will be using the graphical interface WebMO to build organic and inorganic molecules with varying degrees of symmetry. Working together in teams, you will first identify the symmetry elements in a series of molecules, then determine the point group of each. You will then be given several point groups and be asked to develop molecules that align with each using either cyclohexane or benzene as your initial structural backbone.

Activity developed by: Prof. Alex Davis, Cabrini University, 2022. Modified by Kevin Range and Bill Vining, 2024, 2026.

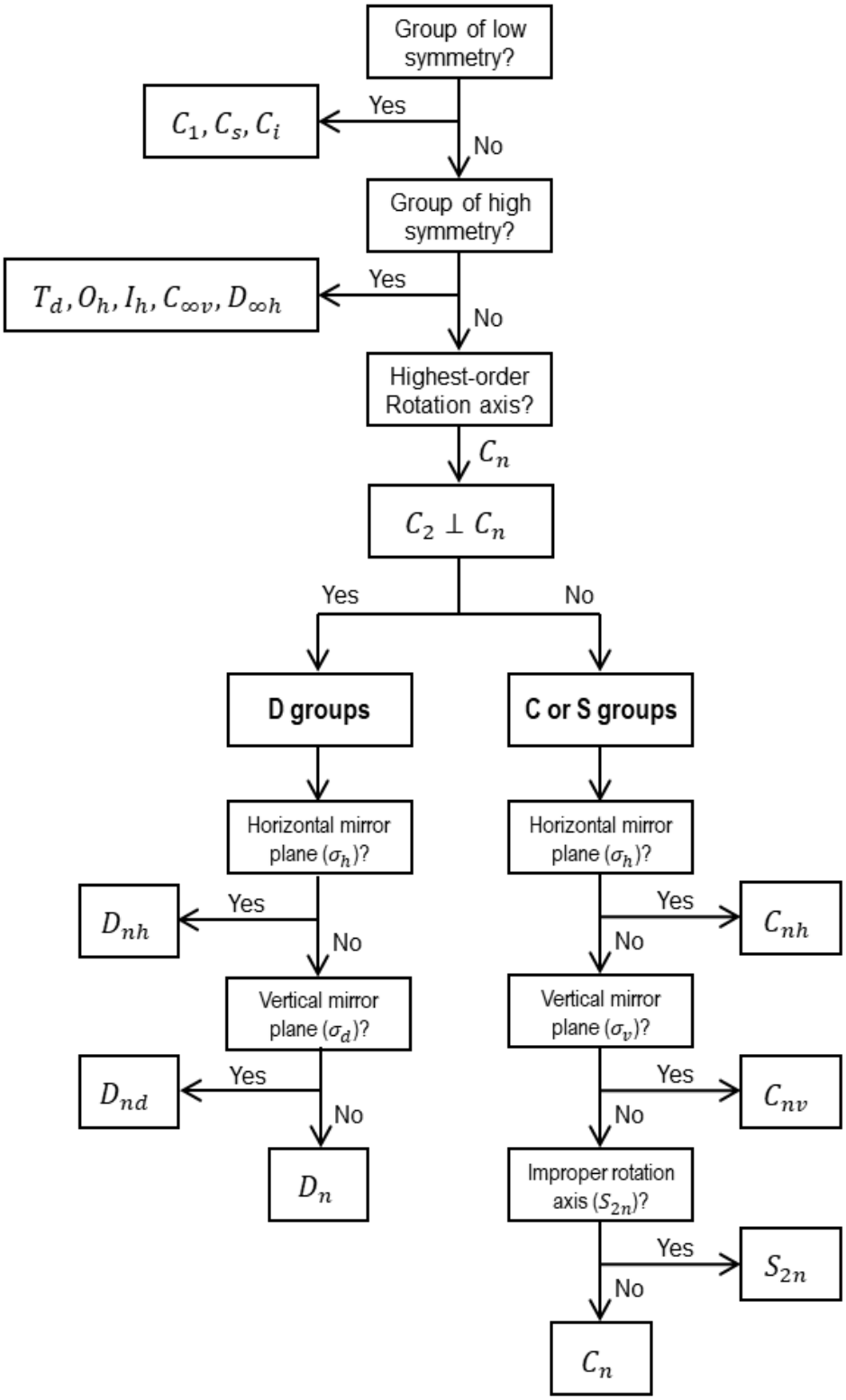


Figure 1. Point group flow chart.

Part 1: symmetry operations and point groups of some molecules

ethane

1. From the WebMO Job Manager choose **New Job > Create New Job.**
2. Click on the  on the left and select Carbon. Then click once in the window to place a carbon atom on the screen.
3. Click on the first carbon, drag to a new location and release the button to drop another carbon that is single bound to the first.
4. Choose **Cleanup > Idealized.** That will cause cleanup to add hydrogen atoms to fill each carbon atom's octet. This will also adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
5. Click on the  on the left to enable you to rotate the molecule.
6. Click on the  on the left to fully symmetrize the molecule. Note: this icon will change the lettering and numbering based on the point group of the current molecule in the build window.
7. Click on the  on the left to show all of the symmetry elements on the molecule.
8. Choose **Calculate > Symmetry > Select Symmetry Elements**. This will open a window that will enable you to select the sets of symmetry elements you would like to see. For each of the following you will need to reopen the window to make each selection.
    - **a.** Select **C3** then click **OK.** This is the principal axis of rotation; it is the C_n axis with the highest n value. Enter C_3 into Table 1 below.
    - **b.** Select **C2** then click **OK**. These are the perpendicular (or subsidiary) C_2 axes. Count them and write that value into the corresponding location in Table 1 below.
    - **c.** Select **S6** then click **OK**. This is the improper axis, which consists of a rotational axis and a mirror plane. Count them and write that value into the corresponding location in Table 1 below.
    - **d.** Select σ then click **OK**. These are the mirror planes. Look for one blue circular plane that is perpendicular to the primary axis. This is referred to as a horizontal mirror plane, if one is present enter 1 into the corresponding location in Table 1 below. Next if there are additional blue circular planes count all of them that are parallel with the primary axis. These are called vertical mirror planes. Write the number you counted into the corresponding location in Table 1 below
    - **e.** Select **i** then click **OK**. This is the inversion center. If one is present enter 1 into the corresponding location in Table 1 below.

f. Use figure 1 and the information you just collected to determine the point group of the molecule. Compare your results with the value displayed on the "Symmetrize" button (D_{3d}) on the left, do they agree?

9. When you are finished collecting data for ethane, from the top tool bar choose **File > New.**

ethene

10. Click on the  on the left and select Carbon. Then click once in the window to place a carbon atom on the screen.
11. Click on the first carbon, drag to a new location and release the button to drop another carbon that is single bound to the first.
12. Click again on the first carbon then drag and release on the second carbon. This will change the single bond to a double bond.
13. Choose **Cleanup > Idealized.** That will cause cleanup to add hydrogen atoms to fill each carbon atom's octet. This will also adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
14. Enter the symmetry data for ethene in Table 1 by repeating steps 5-8 above for this molecule. If one of the components of a-e in step 8 is missing, skip that step and enter a zero in the corresponding location.

1,1-dichloroethene

15. Once you have finished entering in the data to Table 1, click on the  on the left and select Chlorine. Then click once on one of the hydrogen atoms on your ethene molecule. This replaces the hydrogen with a chlorine atom. Click on the other hydrogen atom that is attached to the same carbon as the first. in the window to place a carbon atom on the screen.
16. Choose **Cleanup > Idealized.** This will adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
17. Enter the symmetry data for 1,1-dichloroethene in Table 1 by repeating steps 5-8 above for this molecule. If one of the components of a-e in step 8 is missing, skip that step and enter a zero in the corresponding location.

cis-1,2-dichloroethene

18. Once you have finished entering in the data to Table 1, click on the  on the left and select Hydrogen. Then click once on one of the chlorine atoms on your molecule. This replaces the chlorine with a hydrogen atom. Click again on the  on the left and select Chlorine. Then click once on the

hydrogen atom on the same side of the double bond. This should give you an initial structure for cis-1,2-dichloroethene.

19. Choose **Cleanup > Idealized.** This will adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
20. Enter the symmetry data for this molecule in Table 1.

trans-1,2-dichloroethene

21. Once you have finished entering in the data to Table 1, click on the  on the left and select Hydrogen. Then click once on one of the chlorine atoms on your molecule. This replaces the chlorine with a hydrogen atom. Click again on the  on the left and select Chlorine. Then click once on the hydrogen atom on the opposite side of the double bond. This should give you an initial structure for trans-1,2-dichloroethene.
22. Choose **Cleanup > Idealized.** This will adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
23. Enter the symmetry data for this molecule in Table 1.

cyclopropane

24. When you are finished collecting data for trans-1,2-dichloroethene, from the top toolbar choose **File > New.**
25. Click on the  on the left and select Carbon. Then click once in the window to place a carbon atom on the screen.
26. Click on the first carbon, drag to a new location and release the button to drop another carbon that is single bound to the first.
27. Click again on the first carbon then drag and release at a new location. This will add another carbon atom. Click on the new carbon then drag to and release on the second carbon to form a triangle.
28. Choose **Cleanup > Idealized.** That will cause cleanup to add hydrogen atoms to fill each carbon atom's octet. This will also adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
29. Enter the symmetry data for this molecule in Table 1.

fluorocyclopropane

30. Replace one of the hydrogens on your cyclopropane with fluorine to form fluorocyclopropane.
31. Choose **Cleanup > Idealized.**
32. Enter the symmetry data for this molecule in Table 1.

cis-1,2-difluorocyclopropane

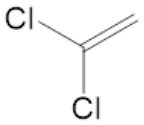
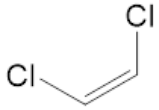
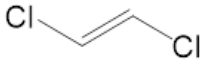
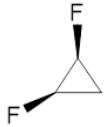
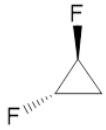
33. Replace another hydrogen on your fluorocyclopropane with fluorine to form cis-1,2-difluorocyclopropane.
34. Choose **Cleanup > Idealized.**
35. Enter the symmetry data for this molecule in Table 1.

trans-1,2-difluorocyclopropane

36. Build trans-1,2-difluorocyclopropane.
37. Choose **Cleanup > Idealized.**
38. Enter the symmetry data for this molecule in Table 1.

In your team, reflect on how adding and moving atoms like chlorine and fluorine affected the symmetry elements that are present in the molecule before moving on to Part 2.

Table 1: Symmetry operations and point groups for predetermined molecules

Molecule	Skeletal Structure	*Primary axis of rotation type (C_n)*	*Number of*				Inversion center (i)	Point Group
			Rotation Axis (C_n, S_n)		Mirror planes (σ)			
			Perpendicular	Improper	v	h		
Ethane		C_3	3 C_2	1 S_6	3	1	1	D_{3d}
Ethene								
1,1-dichloroethene								
Cis-1,2-dichloroethene								
Trans-1,2-dichloroethene								
Cyclopropane								
Fluorocyclopropane								
Cis-1,2-difluorocyclopropane								
Trans-1,2-difluorocyclopropane								

Part 2: Building molecules with a certain point group

Using what you have learned about adjusting substituents on molecules you and your teams will now create molecules using either benzene or cyclohexane as your starting structures that have the point groups listed in Table 2.

39. Instead of building molecules from scratch, we can also download structures from databases using their names. From the top toolbar choose **Lookup > Import by > Name**. This will open a Query structure window. Type "benzene" into the window and click **OK**.
40. Choose **Cleanup > Idealized.** This will adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
41. Repeat the above steps 5-8 for benzene, entering your results into Table 2. If one of the components of a-e in step 8 is missing, skip that step and enter a zero in the corresponding location.
42. From the top toolbar choose **Lookup > Import by > Name**. This will open a Query structure window. Type "cyclohexane" into the window and click **OK**.
43. Choose **Cleanup > Idealized.** This will adjust the bond distances, angles, and dihedral angles for each atom in the molecule.
44. Repeat the above steps 5-8 for cyclohexane, entering your results into Table 2. If one of the components of a-e in step 8 is missing, skip that step and enter a zero in the corresponding location.
45. Using either cyclohexane or benzene as your starting point and chlorine and/or fluorine as substituents build your own molecules that match the point groups listed in table 2.
    a. Make sure you choose **Cleanup > Idealized** after you finish building each molecule.
    b. Fill out the missing information from table 2, including the name of your compounds and their skeletal structures.

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Table 2: Molecules developed based on assigned point groups.

Molecule	Skeletal Structure	*Primary axis of rotation type (C_n)*	*Number of*				Inversion center (i)	Point Group
			Rotation Axis (C_n, S_n)		Mirror planes (σ)			
			Perpendicular	Improper	Vertical	Horizontal		
Benzene								
Cyclohexane								
								D_{3d}
								C_2
								C_{3v}
								D_{2h}
								C_i