Math Methods I
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Groups

Introduction to Groups via Symmetry Groups of Molecules. Determination of the structure of molecules is one of many examples of the use of the group theory. Electronic structure of a molecule can be determined via its geometric structure. In this case, one consider the symmetry of a molecule since it reveals information about its properties (i.e., structure, spectra, polarity, chirality, etc). This process is represented by the following diagram.

$$\begin{tikzcd}
\boxed{\text{Geometry of a molecule}} \arrow[r] & \boxed{\text{Symmetry Group}} \arrow[d] \\
\boxed{\text{Structural Properties}} \arrow[u] & \boxed{\text{Group Representation}} \arrow[l]
\end{tikzcd}$$

Symmetry of a molecule is characterized by the fact that it is possible (theoretically) to carry out **operations** which interchange the position of some (or all atoms) and result in the arrangement of atoms that is indistinguishable from the initial arrangements. These operations are exactly those that we can apply on a model of a molecule so that the resulting molecule appears the same as the original one.

Operations are:

- **rotations** - physically possible, are called proper rotations.
- **reflections** with the respect to a mirror plane or to the center of symmetry - physically impossible, are called improper rotations.

These set of all those operations is called a **group of symmetries**. The features of such group that we are interested in is that

1) **a composite of two operation from the group is again an operation from the group.**

If a and b are two operations, their composite is denoted by $a \cdot b$ or, shorter ab. With this notation, the operations a, b and c of a symmetry group satisfy the **associativity law:**

2) $a(bc) = (ab)c$

There is a distinct element of every group of symmetry, called the **identity element** and denoted by 1. This element corresponds to the operation of not moving the molecule at all (equivalently, the rotation for 0 degrees). This, we have that the rule below holds.

3) $a1 = 1a = a$ for every operation a.

In addition, for every operation a, there is an operation reversing the effect of a. This operation is denoted by a^{-1}. For example, if a is the rotation for α degrees, then a^{-1} is the rotation for α degrees in the opposite direction (equivalently, rotation for $-\alpha$ degrees). The composition of a and a^{-1} is the identity operation.

4) $aa^{-1} = a^{-1}a = 1$.

These four laws are independent of the chemical setting and, as it turned out, there are many other situations in which the set of elements considered satisfies these four laws. So, it turned out that the study of any structure satisfying the above four laws, **a group**, was of interest for many disciplines. The study of group became known as the **group theory**.

History. Historically, group was not defined in the context of chemistry and symmetries of molecules. There are three historical roots of group theory: 1) the theory of algebraic equations, 2) number theory and 3) geometry. Euler, Gauss, Lagrange, Abel and Galois were early researchers in the field of group theory. Galois is honored as the first mathematician linking group theory and field theory, with the theory that is now called Galois theory.

Galois remains an intriguing and unique person in the history of mathematics. The footnote contains some more information from wikipedia.org. [1]

Mathematical Definition of a Group. We revisit the four rules above to present a precise mathematical definition of a group.

A group is a nonempty set G together with an operation $\cdot$ such that the rules A1 to A4, listed below, hold.

[1]

Évariste Galois (October 25, 1811 May 31, 1832) was a French mathematician born in Bourg-la-Reine. He was a mathematical child prodigy. While still in his teens, he was able to determine a necessary and sufficient condition for a polynomial to be solvable by radicals, thereby solving a long-standing problem. His work laid the fundamental foundations for Galois theory, a major branch of abstract algebra, and the subfield of Galois connections. He was the first to use the word "group" as a technical term in mathematics to represent a group of permutations. He died in a duel at the age of twenty.

The night before the duel, supposedly fought in order to defend the honor of a woman, he was so convinced of his impending death that he stayed up all night writing letters to his friends and composing what would become his mathematical testament. Hermann Weyl, one of the greatest mathematicians of the 20th century, said of this testament, "This letter, if judged by the novelty and profundity of ideas it contains, is perhaps the most substantial piece of writing in the whole literature of mankind." In his final papers he outlined the rough edges of some work he had been doing in analysis and annotated a copy of the manuscript submitted to the academy and other papers. On the 30th of May 1832, early in the morning, he was shot in the abdomen and died the following day at ten in the Cochin hospital (probably of peritonitis) after refusing the offices of a priest. He was 20 years old. His last words to his brother Alfred were: "Don't cry, Alfred! I need all my courage to die at twenty."

Galois' mathematical contributions were finally fully published in 1843 when Liouville reviewed his manuscript and declared that he had indeed solved the problem first proposed and also solved by Abel. The manuscript was finally published in the October-November 1846.

A1 The result of operation applied to two elements of G is again an element of G (i.e. if a and b are in G, $a \cdot b$ is also in G). In this case we say that the operation $\cdot$ is **closed**.

A2 Associativity holds: $(a \cdot b) \cdot c = a \cdot (b \cdot c)$ Operation with this property is said to be **associative**.

A3 There is **identity element** 1 so that $a \cdot 1 = 1 \cdot a = a$ for every element a.

A4 Every element a has the **inverse** a^{-1} (i.e. $a \cdot a^{-1} = a^{-1} \cdot a = 1$).

As before, we shorten the notation $a \cdot b$ and write just ab. Also, if G with operation $\cdot$ is a group, we say that G is a group **under operation** $\cdot$.

Examples.

1. The set of real numbers without zero is a group under multiplications. Indeed, A1 holds since if a and b are nonzero real numbers, then ab is also a nonzero real number.

   The associativity $(ab)c = a(bc)$ holds for any nonzero real numbers a, b, c so A2 holds.

   A3 holds since 1 is the identity element: $a1 = 1a = a$ for every element a.

   Every element a has the inverse $\frac{1}{a}$ such that $a\frac{1}{a} = \frac{1}{a}a = 1$. So, A4 holds.

   Note that the rational or complex numbers without zero also form groups under multiplication.

   The set of all real numbers (with zero left in it) is not a group under multiplication because A4 fails: there is no solution of the equation $0x = 1$ (i.e. we cannot divide with 0) so 0 does not have an inverse.

2. The set of real numbers under addition is a group. This example illustrates that the operation in a specific group can be denoted differently than $\cdot$ and should not be associated only with multiplication. The laws A1–A4 remain to hold regardless of the change in notation. Indeed, A1 holds since if a and b are real numbers, then $a + b$ is also a real number.

   The associativity $(a + b) + c = a + (b + c)$ holds for any real numbers a, b, c so A2 holds.

   A3 holds since 0 is the identity element: $a + 0 = 0 + a = a$ for every element a.

   Every element a has the inverse $-a$ such that $a + (-a) = (-a) + a = 0$. So, A4 holds.

   Note that the integer, rational, or complex numbers are also a group under addition.

3. Vectors in the xy-plane (or in xyz-space) form a group under addition. In addition, real valued matrices form a group under addition.

4. The set of invertible real valued functions forms a group under the composition of functions. In all of the previous examples, the **commutativity law** ($ab = ba$ for all a, b) holds. In this example, it does not hold. For example, if $f(x) = 2x$ and $g(x) = x - 1$. Then $f(g(x)) = 2(x - 1) = 2x - 2$, $g(f(x)) = (2x) - 1 = 2x - 1$, and so $f \circ g \neq g \circ f$. Similarly, the invertible real valued matrices form a group under the matrix multiplication. The commutative law also fails in this group.

All the groups in the above examples have infinitely many elements. We present many examples of groups with finitely many elements also. Let us introduce some related definitions.

The order of a group. The order of a group element. If a group G has n elements, we say it has **order** n. If an element a is such that $a^n = 1$ and $a^m \neq 1$ for any $m < n$, we say that a has **order** n.

Non-examples. Let us present some "non-examples" (i.e., examples of sets with operations which fail some of the rules A1 to A4) next. The set of positive integers is not closed under subtraction because, for example, 2 and 3 are positive integers and $2 - 3$ is not. So, A1 fails.

The set of integers is not associative under subtraction since

$$a - (b - c) = a - b + c \neq a - b - c = (a - b) - c$$

so A2 fails.

Positive integers do not satisfy even A3 under addition because 0 is not a positive integer.

Nonnegative integers are not a group under addition since A4 does not hold. For example, 2 does not have an inverse because -2 is not a positive integer.

The axiom A4 also fails for the set of integers without zero under multiplication. Indeed, 2 does not have an inverse since $\frac{1}{2}$ is not a nonzero integer.

Why A1–A4? Let us expand on the meaning of the axioms A1 to A4. The axiom A1 is necessary to avoid situations as in the example with positive integers and subtraction.

The axiom A2 enables us not to use the parenthesis. So, we can shorten $(ab)c = a(bc)$ simply to abc. This rule also enables us to write long formulas like $a(b((cd)e)(fg))$ simply as $abcdefg$.

The axioms A2, A3, and A4 enable us to "divide" i.e. these rules guarantees that the equations $ax = b$ and $ya = b$ have unique solutions in G for all a and b. Indeed, to solve the first equation, we can use A4 to ensure that a^{-1} exists and then multiply the equation on the left with a^{-1}. We use A2 to write the left side $a^{-1}(ax)$ as $(a^{-1}a)x$, A4 to have this as $1x$ and A3 to have this as x. Since the right side is $a^{-1}b$, $x = a^{-1}b$ is a solution.

Uniqueness follows from the left **cancellation law:** $\underline{ax = ay \quad \text{imply} \quad x = y}$.

Indeed, assuming that $ax = ay$, we can use A4 to ensure the existence of a^{-1} and multiply the equation on the left with a^{-1} to get $a^{-1}(ax) = a^{-1}(ay)$. Then we can use A2 to regroup the terms to get $(a^{-1}a)x = (a^{-1}a)y$. Using A4, we have that $1x = 1y$ and, finally, using A3, we conclude that $x = y$.

Similarly, by multiplying the equation $ya = b$ on the right with a^{-1} and using the right cancellation law, one shows that ba^{-1} is a unique solution of this equation.

The converse holds as well: a set G satisfying A1, A2 and the rule

D For all a and b from G, the equations $ax = b$ and $xa = b$ have unique solutions in G.

satisfies the rules A3 and A4 as well. Indeed, A3 holds because 1 is the solution of the equation $ax = a$ for an element a (one would still have to show that $ax = a$ and $bx = b$ produce the same solution for different a and b). The axiom A4 holds since, for every element a, the solution of the equation $ax = 1$ is a^{-1} (one would still have to show that a^{-1} is also the solution of $ya = 1$).

Cayley Tables. The fact that the equations of the form $ax = b$ and $ya = b$ have unique solutions in a group provides a very easy way to check if a given finite set of elements forms a group under a given operation. Such operation on a finite set of elements is frequently given by a table listing the result of the operation for each pair of elements. Such table is called a **Cayley table**, named after the mathematician Arthur Cayley. Cayley table is a generalization of the **multiplication table** used for multiplication of integers: it is a grid where rows and columns are headed by the elements to multiply, and the entry in each cell is the product of the column and row headings.

For example, following is a Cayley table on the set of three elements a, b, c.

$\cdot$	a	b	c
a	a	b	a
b	c	a	b
c	c	c	b

Let us look at the part of the table without column and row headings. Note that the first row represents different results of the multiplication from the left with a. But in the first row, there is no element c. That means that the equation $ax = c$ has no solution. Hence, this table does not represent a group. Similarly, note that in the first (non-headed) column, there is not element b present. As a consequence, the equation $ya = b$ has no solution.

From this example, we can conclude that a necessary condition for a Cayley table to represent a group is that in every row and column each element appear at least once. If some elements appears twice, then the cancellation law does not hold so

1) Every element appears exactly once in every row and every column.

Also,

2) There has to be an element such that the row and column determined by that elements are the same as the heading row and column. In this case, that element is the identity.

If a Cayley table of a set G satisfies rules 1 and 2, then G satisfies A1, A3, A4. Associativity law A2 is hard to check using Cayley table. Checking associativity boils down to checking all the possible triples of elements a, b, c satisfy the rule $(ab)c = a(bc)$.

An example of a Cayley table of a set of three elements that is a group is

$\cdot$	a	b	c
a	a	b	c
b	b	c	a
c	c	a	b

In this example, a is the identity, and b and c are mutually inverse to each other.

A group is called **abelian** if it satisfies the commutative law

$$ab = ba.$$

We have seen many examples of abelian groups and some examples of groups that are not abelian. If a group is finite, one can easily check if it is abelian or not using its Cayley table: you simply check if the table is symmetric with respect to the main diagonal. Using this rule, we conclude that the group with the above Cayley table is abelian.

Groups with 2 elements. Let us use Cayley table to try to determine all possible groups with 2 elements. As one of them has to be identity, let us denote that element by 1 and the other element by a. Since $a1 = 1a = a$, the result of aa cannot be a so it has to be 1. Hence,

$\cdot$	1	a
1	1	a
a	a	1

is the resulting table.

Note that this is the only possible way we could fill the table. This means that every other group of two elements is going to have the multiplication table matching this multiplication table. For example, if we consider a group with two elements c, d and c is the identity, then $cd = d$ implies that dd cannot be d so it is c. Hence, the multiplication table is

$\cdot$	c	d
c	c	d
d	d	c

Thus, the only difference between the two groups are the names we assigned to the elements. The correspondence $1 \leftrightarrow c$ and $a \leftrightarrow d$ is such that each element of one group corresponds to a unique element of the other group and such that the Cayley tables match. Such correspondence is an example of a **group isomorphism**. If a group isomorphism exists, we say that two groups are **isomorphic**. Isomorphic groups have all relevant properties the same (including a matching multiplication operations), so mathematicians are often considering them as one same group. One of the most important questions in group theory is to determine if a given two groups are isomorphic or not. In chemistry, isomorphic groups are sometimes referred to as isomorphous groups.

A group isomorphism preserves all the group properties. This gives you useful criterion for determining that two groups are not isomorphic.

- To demonstrate that **two groups are not isomorphic**, you can find a property they do not share. For example, if the groups have a different number of elements, or if one is abelian and the other is not, then those groups are not isomorphic.

On the other hand,

- to demonstrate that **two groups are isomorphic**, you can match their elements and show that the matching preserves the Cayley table. We shall see later that if two groups have the same presentation, then they are isomorphic.

We present a more concrete example of a group with two elements next. Let us consider, the group of two integers 1 and -1 under the multiplication. The multiplication table

$\cdot$	1	-1
1	1	-1
-1	-1	1

shows that this group is also isomorphic to the above group with elements a and b.

Yet another example is the group of remainders when dividing with 2. Note that when any integer is divided by 2, the remainder is either 0 or 1. Thus $1+0 = 0+1 = 1$, $0+0 = 0$. As 1+1=2 and 2 has remainder 0 when divided by 2, we have that 1+1=0. Thus, we have the following table.

$+$	0	1
0	0	1
1	1	0

All of the above groups are isomorphic with each other. We use the notation C_2 to represent any of the (mutually isomorphic) groups with two elements.

Groups with 3 elements. Let us consider the groups of three elements. As one of the three elements has to be identity, let us denote elements by 1, a and b and let us start filling the Cayley table as follows.

$\cdot$	1	a	b
1	1	a	b
a	a		
b	b		

If we put 1 in the first empty place in the second row of the table (again the rows are counted without the heading elements), then we would have to put b in the last free place in the second row in order not to violate the rule that each element in each row appears exactly once. But then b would appear twice in the last column, so we cannot fill the table this way.

This mean that the second row has to be $a, b, 1$ and this uniquely determines the last row and hence the entire table. So, the following is the complete Cayley table.

$\cdot$	1	a	b
1	1	a	b
a	a	b	1
b	b	1	a

Since $b = a^2$, we can also write this table simpler as follows.

$\cdot$	1	a	a^2
1	1	a	a^2
a	a	a^2	1
a^2	a^2	1	a

Since this is the only way how we can fill the table, every other group with three elements is isomorphic to this one (in particular, the group from the example on page 5 is isomorphic to this one). Another group of three elements (also isomorphic to the one above) can be obtained considering the remainders when dividing with 3, similarly as in the example with the two-element group. Any integer has a remainder when divided by 3 either 0, 1 or 2. So, we take these three elements to be the elements of the group.

To obtain the Cayley table, note that the elements add considering the remainder of their sum when dividing by 3. For example 2+2=4 which has remainder 1 when divided by 3, so 2+2=1. Thus, we have the following table.

$+$	0	1	2
0	0	1	2
1	1	2	0
2	2	0	1

Note that the identity element here is 0, not 1 since we are using the additive, not multiplicative notation. Analogously to the 2-element groups, the notation C_3 is used to denote any group with 3 elements.

As we have seen, there is just one (isomorphism type of a) group with two and just one (isomorphism type of a) group with three elements. Considering groups with four elements later on, we arrive to a more interesting situation: there are two groups of order 4 which are not isomorphic to each other. Before those examples, let us generalize the examples with C_2 and C_3 to define the cyclic group C_n of order n.

Cyclic groups $\mathbf{C_n}$. Cyclic groups are those that are generated with a single element. This means that every other element can be represented by that single element or its inverse. For example, the set of integers under addition is generated by 1 because every integer is a sum of copies of 1 or -1 (for example 3=1+1+1 and $-3 = (-1) + (-1) + (-1)$). It turns out that any infinite cyclic groups is isomorphic to this one.

The group C_n is defined as generated by a single element a which satisfies the relation $a^n = 1$. We write these requirements shorter as

$$C_n = \langle a \mid a^n = 1 \rangle.$$

by listing the generator before the symbol | and listing the defining relation after the symbol |. This means that C_n consists of n elements $1, a, a^2, \ldots, a^{n-1}$ – not more since all higher powers of a can reduce to one of these elements by using the relation $a^n = 1$. This relation also implies that $1 = a^n = aa^{n-1}$ so $a^{-1} = a^{n-1}$. Because of this, the negative powers of a can also be reduced to one of the n elements listed above. Thus, C_n has order n. The multiplication table is completely determined by the relation $a^n = 1$.

For example, C_5 consists of five elements $a^0 = 1, a, a^2, a^3, a^4$. The Cayley table is the left table below. This group is isomorphic to the group of remainders when dividing integers by 5. The table of this groups is on the right side below.

$\cdot$	1	a	a^2	a^3	a^4
1	1	a	a^2	a^3	a^4
a	a	a^2	a^3	a^4	1
a^2	a^2	a^3	a^4	1	a
a^3	a^3	a^4	1	a	a^2
a^4	a^4	1	a	a^2	a^3

$+$	0	1	2	3	4
0	0	1	2	3	4
1	1	2	3	4	0
2	2	3	4	0	1
3	3	4	0	1	2
4	4	0	1	2	3

The correspondence $1 \mapsto 0, \quad a \mapsto 1, \quad a^2 \mapsto 2, \quad a^3 \mapsto 3$ and $a^4 \mapsto 4$ is an isomorphism between the two groups above. This isomorphism can be shortly represented by $a^i \mapsto i$ for $i = 0, 1, \ldots, 4$.

Using the rule that $a^k a^l = a^{k+l} = a^{l+k} = a^l a^k$ once can conclude that every cyclic group is abelian.

Presentation of a group. The notation $C_n = \langle a \mid a^n = 1 \rangle$ is an example of a group presentation. In general, we can use the notation

$$\langle \text{ list of generators } \mid \text{ list of relations on the generators } \rangle,$$

called a **group presentation**, to represent a group. Note that a presentation is not unique.

Groups with 4 elements. Let us return to the groups with 4 elements now. We know that C_4 is an example of a group with four elements. To determine if any other (nonisomorphic) groups with four elements exist, let us denote the elements by $1, a, b, c$ and let us explore the possible ways of filling the multiplication table. Since $aa \neq a$ (otherwise a appears twice in the row and column led by a) the options for aa are b, c or 1. The first two choices determine the rest of the table uniquely. If $a^2 = b$ then $a^3 = c$ (try to fill the table and convince yourself of this) and $ac = a^4 = 1$. So, this group can be generated by the single element a which satisfies the relation $a^4 = 1$. Thus, it is (isomorphic to) C_4.

If $a^2 = c$, the rest of the table implies that $a^4 = c^2 = 1$ and $a^3 = ac = b$. Hence, this group is also generated by the single generator a which satisfies the relation $a^4 = 1$ so it is also isomorphic to C_4.

If $a^2 = 1$, then the rest of the table depend on whether b^2 is a or 1. If it is a, then $c = ab = b^2 b = b^3$ and $1 = aa = b^2 b^2 = b^4$ so this group can be generated by b only ($a = b^2$ and $c = b^3$) and this generator also satisfies the relation $b^4 = 1$ so this group has presentation $\langle b \mid b^4 = 1 \rangle$ which is also isomorphic to C_4.

The last remaining choice is when $a^2 = 1$ and $b^2 = 1$. In this case, $c = ab$ and so this group can be generated by two generators, a and b and has the following table.

$\cdot$	1	a	b	c
1	1	a	b	c
a	a	1	c	b
b	b	c	1	a
c	c	b	a	1

$c = ab \;\Rightarrow$

$\cdot$	1	a	b	ab
1	1	a	b	ab
a	a	1	ab	b
b	b	ab	1	a
ab	ab	b	a	1

This group is not isomorphic to C_4 because C_4 has an element whose square is not 1 and the squares of all elements of this group are 1 (1 is on the main diagonal of the table above). This means that there is one more groups of order 4, not isomorphic to C_4. We denote this group by $C_2 \times C_2$ and say that it is a direct product of two copies of the cyclic group C_2. We consider the direct product in more details next.

Direct Product of Groups and their presentations. Recall that the xy-plane is obtained by considering the ordered pairs (x, y) of real numbers. We can consider it to be a *direct product* of two copies of the set of real numbers: the first coordinate of an ordered pair is a real number considered as an element of the first copy and the second coordinate is a real number considered as an element of the second copy. Analogously, a new group can be obtained by considering ordered pairs of elements from two other groups. More precisely, if G_1 and G_2 are two groups, we can define a new group $G = G_1 \times G_2$ by considering the elements of G to be the ordered pairs (g_1, g_2) where g_1 is from G_1 and g_2 is from G_2. The operation in G is defined by the following:

$$(g_1, g_2) \cdot (h_1, h_2) = (g_1h_1, g_2h_2).$$

If G_1 has n elements and G_2 has m elements, then $G_1 \times G_2$ has mn elements.

If any of the groups G_1 or G_2 is infinite, then $G_1 \times G_2$ is infinite. The xy-plane, for example, can be thought of as a direct product of one copy of real numbers (under addition) with another copy of real numbers. Note that this groups is the same as the group of vectors in the xy-plane under addition. We can consider the direct product of xy-plane and another copy of real numbers to get the xyz-space.

Given presentations of G_1 and G_2, a presentation of $G_1 \times G_2$ is obtained using the following rules.

- The generators of $G_1 \times G_2$ are the generators G_1 and the generators of G_2.
- The relations on $G_1 \times G_2$ are those of G_1, those of G_2, plus the relations that assert that the generators of G_1 commute with the generators of G_2.

Example 1. Write a presentation and the Cayley table of the group $C_2 \times C_2$. Then note the isomorphism of this group and the one with 4 elements not isomorphic to C_4.

Solution. Let us consider the first copy of C_2 to have the presentation $\langle a \mid a^2 = 1\rangle$ and the second one to have the presentation $\langle b \mid b^2 = 1\rangle$. Thus, the product $C_2 \times C_2$ can be represented by

$$\langle a, b \mid a^2 = 1, b^2 = 1, ab = ba\rangle.$$

So, this group has 4 elements $1, a, b$, and ab as any other "word" in two letters a and b can be written as one of those 4 using the above relations (for example $ababb = a^2b^3 = 1b = b$ and $abbaaaba = a^5b^3 = ab$). The Cayley table for this group matches the second table in the section on groups of order 4

$\cdot$	1	a	b	ab
1	1	a	b	ab
a	a	1	ab	b
b	b	ab	1	a
ab	ab	b	a	1

. Thus, we say that there are two nonisomorphic groups of order 4, C_4 and $C_2 \times C_2$.

We can also think of $C_2 \times C_2$ as the set of the ordered pairs where the first entry is 1 or a and the second entry is 1 or b. This representation yields a group isomorphic to the one with the table above by the correspondence

$$1 \mapsto (1, 1), \quad a \mapsto (a, 1), \quad b \mapsto (1, b), \quad \text{and} \quad ab \mapsto (a, b).$$

You can also think of the ordered pairs with 0 or 1 as the entries and the addition as your operation. So, $(0,1)+(1,1)$, for example, is equal to $(0+1,1+1)=(1,0)$. This group is isomorphic to $C_2 \times C_2$ and the map given by $1 \mapsto (0,0)$, $a \mapsto (1,0)$, $b \mapsto (0,1)$, and $ab \mapsto (1,1)$ is an isomorphism.

Example 2. Write down a presentation and the Cayley table of the group $C_3 \times C_2$ and show that it is isomorphic to C_6.

Solutions. The group $C_3 \times C_2 = \langle a \mid a^3 = 1\rangle \times \langle b \mid b^2 = 1\rangle$ can be presented as

$$\langle a, b \mid a^3 = 1, b^2 = 1, ab = ba\rangle.$$

So, this group has 6 elements $1, a, a^3, b, ab, a^2b$ as any other ”word” in two letters a and b can be written as one of those 6 using the above relations. Try to fill the Cayley table using the presentation above and check that it matches the following table.

$C_3 \times C_2$	1	a	a^2	b	ab	a^2b
1	1	a	a^2	b	ab	a^2b
a	a	a^2	1	ab	a^2b	b
a^2	a^2	1	a	a^2b	b	ab
b	b	ab	a^2b	1	a	a^2
ab	ab	a^2b	b	a	a^2	1
a^2b	a^2b	b	ab	a^2	1	a

Let us consider the cyclic group of order 6 $C_6 = \langle c \mid c^6 = 1\rangle$. We claim that these two groups are isomorphic. To show that, note that the element ab has order 6. Indeed

$(ab)^0$	$(ab)^1$	$(ab)^2$	$(ab)^3$	$(ab)^4$	$(ab)^5$	$(ab)^6$
1	ab	a^2	b	a	a^2b	1

Then note that this can be matched with the powers of element c in $C_6 = \langle c \mid c^6 = 1\rangle$.

$(ab)^0$	$(ab)^1$	$(ab)^2$	$(ab)^3$	$(ab)^4$	$(ab)^5$	$(ab)^6$
1	ab	a^2	b	a	a^2b	1
1	c	c^2	c^3	c^4	c^5	c^6

Comparing the Cayley's tables shows that the pairing of the elements above really is the isomorphism of the two groups.

$C_3 \times C_2$	1	ab	a^2	b	a	a^2b
1	1	ab	a^2	b	a	a^2b
ab	ab	a^2	b	a	a^2b	1
a^2	a^2	b	a	a^2b	1	ab
b	b	a	a^2b	1	ab	a^2
a	a	a^2b	1	ab	a^2	b
a^2b	a^2b	1	ab	a^2	b	a

C_6	1	c	c^2	c^3	c^4	c^5
1	1	c	c^2	c^3	c^4	c^5
c	c	c^2	c^3	c^4	c^5	1
c^2	c^2	c^3	c^4	c^5	1	c
c^3	c^3	c^4	c^5	1	c	c^2
c^4	c^4	c^5	1	c	c^2	c^3
c^5	c^5	1	c	c^2	c^3	c^4

The scenarios from the previous two examples contrast each other

$$C_3 \times C_2 \cong C_6 \quad \text{while} \quad C_2 \times C_2 \ncong C_4.$$

This indicates a need to be able to answer the following questions.

Which conditions on m and n ensure that $C_m \times C_n$ isomorphic to C_{mn}?
Which conditions ensure that $C_m \times C_n$ is not isomorphic to C_{mn}?

The following claim answers both questions.

$C_m \times C_n$ is isomorphic to C_{mn} if and only if the greatest common divisor of m and n is 1 (i.e. m and n do not have any common factors other than 1).

To prove this claim, you can argue as we did in two examples above:

- If m and n do not have any common factors other than 1, the element ab has order mn so you can define the isomorphism by mapping $ab \mapsto c$. Note that this determines the images of the rest of the elements just like in the example with $m = 3$ and $n = 2$.

- If m and n have the largest common divisor $d > 1$, then the group $C_m \times C_n$ does not have an element of order mn (that is, all its elements are of order smaller than mn). On the other hand, the generator c of C_{mn} has the order mn.

This claim makes possible to determine all the isomorphism classes of abelian groups of certain (finite) order. We illustrate that by the following example.

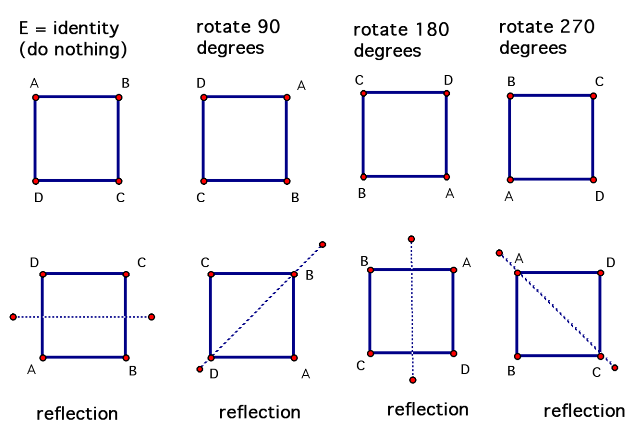
Example 3. Determine which of the following groups are isomorphic.

$$C_{24}, \quad C_{12} \times C_2, \quad C_8 \times C_3, \quad C_6 \times C_4, \quad C_3 \times C_4 \times C_2, \quad C_6 \times C_2 \times C_2, \quad C_3 \times C_2 \times C_2 \times C_2$$

Solution. Note that $24 = 2^3 \cdot 3$ Since any power of 2 and 3 do not have any common factor other than 1, C_3 can be combined with any group of $C_2 \times C_2 \times C_2$, $C_4 \times C_2$, or C_8, creating isomorphic pairs of groups. Any of these three groups, on the other hand, are not isomorphic because 2 and any power of 2 have a common divisor 2 (so not only 1). Thus, there are three classes of abelian groups of order 24 such that the groups in same class are isomorphic and any two groups from two different classes are not isomorphic.

1.	$C_3 \times C_2 \times C_2 \times C_2$	$\cong C_6 \times C_2 \times C_2$	
2.	$C_3 \times C_4 \times C_2$	$\cong C_{12} \times C_2$	$\cong C_6 \times C_4$
3.	$C_3 \times C_8 \cong C_{24}$		

Dihedral Group D_n and its presentation. Dihedral groups are groups of symmetries of regular polygons. The group of symmetries of a regular polygon of n sides is denoted by D_n.



For example, let us consider a square. The symmetries of a square are: rotations for 0, 90, 180 and 270 degrees, reflections with respect to diagonals and x and y axes (if the square is centered at the origin so that the sides are parallel to x or y axis). Clearly, the rotation for 0 degrees is the identity, let us denote it with 1. If we denote the rotation for 90 degrees by a, then the rotations by 180 and 270 degrees are a^2 and a^3 and then $a^4 = 1$.

Let us denote the reflection with respect to y-axis by b. Then $b^2 = 1$, ab is reflection with respect to the main diagonal, a^2b is reflection with respect to x-axis and a^3b is reflection with respect to the non-main diagonal. So, all the symmetries of the square can be written via a and b. This means that a and b are generators of D_4. Also, note that $ba = a^3b$.

Since ba is the reflection with respect to non-main diagonal, it is different than ab, the reflection with respect to main diagonal. So, D_4 is not abelian.

The equations $a^4 = 1$, $b^2 = 1$, and $ba = a^3b$ on the generators a and b completely determine the Cayley table of D_4. This means that the group D_4 can be given by the presentation

$$\langle a, b \mid a^4 = 1, \quad b^2 = 1, \quad ba = a^3b\rangle.$$

Using this presentation, we can fill the table.

$\cdot$	1	a	a^2	a^3	b	ab	a^2b	a^3b
1	1	a	a^2	a^3	b	ab	a^2b	a^3b
a	a	a^2	a^3	1	ab	a^2b	a^3b	b
a^2	a^2	a^3	1	a	a^2b	a^3b	b	ab
a^3	a^3	1	a	a^2	a^3b	b	ab	a^2b
b	b	a^3b	a^2b	ab	1	a^3	a^2	a
ab	ab	b	a^3b	a^2b	a	1	a^3	a^2
a^2b	a^2b	ab	b	a^3b	a^2	a	1	a^3
a^3b	a^3b	a^2b	ab	b	a^3	a^2	a	1

Every dihedral group has an analogous presentation. The group D_n has two generators a, the rotation for $360/n$ degrees, and b, reflection with respect to y axis, and it satisfies $a^n = 1$, $b^2 = 1$, $ba = a^{n-1}b$. Thus,

$$D_n = \langle a, b \mid a^n = 1, \quad b^2 = 1, \quad ba = a^{n-1}b\rangle.$$

As a large percentage of point groups encountered are cyclic, dihedral, product of two cyclic or product of a cyclic and a dihedral, let us look more closely to those examples.

Group	notation	no. of el.	presentation
Cyclic (order n)	C_n	n	$\langle a \vert a^n = 1\rangle$
Product of 2 cyclic	$C_n \times C_m$	mn	$\langle a, b \vert a^n = b^m = 1, ba = ab\rangle$
Dihedral	D_n	$2n$	$\langle a, b \vert a^n = b^2 = 1, ba = a^{n-1}b\rangle$
Product of D_n and C_m	$D_n \times C_m$	$2nm$	$\langle a, b, c \vert a^n = b^2 = c^m = 1, ba = a^{n-1}b, ca = ac, bc = cb\rangle$

We are specially interested in the case when $m = 2$ both when considering $C_n \times C_m$ and $D_n \times C_m$.

We should also note the distinction between $C_n \times C_2$ and D_n. Both of these two groups have $2n$ elements. If $n > 2$, then they are not isomorphic as $C_n \times C_2$ is abelian, while D_n is not ($ba = a^{n-1}b \neq ab$). If $n = 2$, then D_2 and $C_2 \times C_2$ are isomorphic since they can both be presented by $\langle a, b \mid a^2 = 1, b^2 = 1, ba = ab\rangle$.

Example 4. Write down a presentation of $D_3 \times C_2$ and list its elements.

Solution. Since $D_3 = \langle a, b \mid a^n = b^2 = 1ba = a^2b\rangle$ and $C_2 = \langle c \mid c^2 = 1\rangle$, $D_3 \times C_2$ can be presented by

$$\langle a, b, c \mid a^n = b^2 = c^2 = 1, ba = a^2b, ac = ca, bc = cb\rangle.$$

So, this group has 12 elements: six elements of dihedral group $1,\ a,\ a^2,\ b,\ ab,\ a^2b$ and those six elements multiplied by c, resulting in the following six elements $c, ac, a^2c, bc, abc, a^2bc$. Note that any other other "word" in three letters a, b and c can be written as one of those 12 using the above relations.

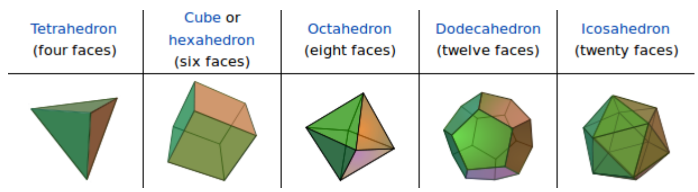
Symmetric Groups. Let us consider the set of three elements $1, 2,$ and 3. Let us look at all the possible permutations of this set (i.e. one-to-one mappings of this set onto itself). As when the symmetries of polygons were considered, the product of two such mappings is their composition. There are six such mappings, mapping $(1, 2, 3)$ to

$$(1, 2, 3),\ (1, 3, 2),\ (2, 1, 3),\ (2, 3, 1),\ (3, 1, 2),\ \text{and } (3, 2, 1)$$

respectively. If we consider these mappings as functions, the operation of function composition makes this set into a group. This groups is called the symmetric group on three letters and it is denoted by S_3. Analogously, the permutations on n elements form a group denoted by S_n. S_n has $n!$ elements.

Symmetric groups are especially important in group theory because of the Cayley's theorem stating that every group can be represented as a subgroup of some symmetric group. There is another important class of groups related to symmetric groups called alternating groups A_n. One of the project topics focuses on the alternating groups A_n.

Platonic or regular solids and their symmetry groups. Platonic solids are convex polyhedra with equivalent faces composed of congruent convex regular polygons. Euclid proved that there are exactly five such solids: the cube, dodecahedron, icosahedron, octahedron, and tetrahedron.



Plato [2] related these geometrical shapes to classical elements. There are just five of these regular solids due to some space limitations that reduce the number of regular solids to only five.

The groups of symmetries of these Platonic solids are the tetrahedral T_d, the octahedral O_h, and the icosahedral group I_h.

The **tetrahedral group** T_d is the group of symmetries of the tetrahedron. It has order 24 and is isomorphic to the group S_4.

[2]**History.** (from wikipedia) The Platonic solids are named after Plato, who wrote about them in Timaeus. Plato learned about these solids from his friend Theaetetus. Plato conceived the four classical elements as atoms with the geometrical shapes of four of the five platonic solids that had been discovered by the Pythagoreans (in the Timaeus). These are, of course, not the true shapes of atoms; but it turns out that they are some of the true shapes of packed atoms and molecules, namely crystals: The mineral salt sodium chloride occurs in cubic crystals, fluorite (calcium fluoride) in octahedra, and pyrite in dodecahedra.

This concept linked fire with the tetrahedron, earth with the cube, air with the octahedron and water with the icosahedron. There was intuitive justification for these associations: the heat of fire feels sharp and stabbing (like little tetrahedra). Air is made of the octahedron; its minuscule components are so smooth that one can barely feel it. Water, the icosahedron, flows out of one's hand when picked up, as if it is made of tiny little balls. By contrast, a highly un-spherical solid, the hexahedron (cube) represents earth. These clumsy little solids cause dirt to crumble and breaks when picked up, in stark difference to the smooth flow of water.

The fifth Platonic Solid, the dodecahedron, Plato obscurely remarks, "...the god used for arranging the constellations on the whole heaven" (Timaeus 55). He didn't really know what else to do with it. Aristotle added a fifth element, aithêr (aether in Latin, "ether" in English) and postulated that the heavens were made of this element, but he had no interest in matching it with Plato's fifth solid.

The **icosahedral group** I_h is the group of symmetries of the icosahedron and dodecahedron having order 120, equivalent to the group direct product $A_5 \times C_2$ of the alternating group A_5 and the cyclic group C_2.

The **octahedral group** O_h is the group of symmetries of the octahedron and the cube. It is isomorphic to $S_4 \times C_2$ and has order 48.

There are many other classes of groups but we are focused on those that appear in chemistry when considering groups of symmetries of molecules.

Finding a good classification for groups (i.e. finding classes that can describe various types of groups well) and finding a good way to represent various abstract groups are two very difficult tasks of the group theory. The group representation theory is a subfield of group theory that deals with these issues.

Symmetry (Point) Groups of Molecules

In the introductory section, we introduced a point group as a group of symmetry operations of a molecule, rotations and reflections. The operation in a point group is a composition of two operation, the action resulted in applying one symmetry followed by another, resulting in yet another symmetry.

There is a step-by-step algorithm that assigns a molecule to a point group and some of you may have covered this process in a chemistry course. Because of this, we present the notation used in chemistry as well as in mathematics.

Operation	Chemistry notation
Identity, rotation for 0 degrees	Identity E
Rotation by $\frac{360}{n}$ degrees	Proper axis C_n
Reflection with respect to a plane (horizontal, vertical, dihedral)	Symmetry plane σ (σ_h, σ_v, σ_d)
Reflection with respect to the origin	Inversion center i
Rotation for $\frac{360}{n}$ degrees followed by the reflection with respect to the horizontal plane	Improper axis S_n

When imagining the **horizontal** plane of symmetry, one can imagine that the molecule model can be floating on water so that exactly half is submerged and the submerged and above-water halves are mapped to each other by the reflection with respect to the water surface. In this case, a **vertical** plane is a plane perpendicular to the water surface.

The table below summarizes chemistry names for all possible point groups.

Type of point group	Chemistry notation
cyclic	C_n
cyclic with horizontal plane	C_{nh}
cyclic with vertical plane	C_{nv}
non-axial	C_i, C_s
dihedral	D_n
dihedral with horizontal plane	D_{nh}
dihedral with plane between axes	D_{nd}
improper rotation	S_{2n}
cubic groups	$I, I_h, O, O_h, T, T_h, T_d$
linear	$C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}$

As we can see from the previous two tables, the same letter is used to denote both a group and its element (often generator) in chemistry. For example, a cyclic group of order n is denoted by C_n and its generator, the rotation for $\frac{360}{n}$ degrees is also denoted by C_n. One should keep this is mind always when working with the point groups using the chemistry notation.

In this course, we are interested both in understanding the mathematical structure of point groups as well as the process of assigning one to a given molecule. The following table addresses the first goal.

Chem.	Math.	no. of el.	presentation
C_n	C_n	n	$\langle a \mid a^n = 1\rangle$
C_{nh}	$C_n \times C_2$	$2n$	$\langle a, b \mid a^n = b^2 = 1, ba = ab\rangle$
C_{nv}	D_n	$2n$	$\langle a, b \mid a^n = b^2 = 1, ba = a^{n-1}b\rangle$
C_i, C_s	C_2	2	$\langle b \mid b^2 = 1\rangle$
D_n	D_n	$2n$	$\langle a, b \mid a^n = b^2 = 1, ba = a^{n-1}b\rangle$
D_{nh}	$C_{nv} \times C_2 = D_n \times C_2$	$4n$	$\langle a, b, c \mid a^n = b^2 = c^2 = 1, ba = a^{n-1}b, ca = ac, bc = cb\rangle$
D_{nd}	D_{2n}	$4n$	$\langle a, b \mid a^{2n} = 1, b^2 = 1, ba = a^{2n-1}b\rangle$
S_{2n}	C_{2n}	$2n$	$\langle a \mid a^{2n} = 1\rangle$
I	A_5	60	$\langle a, b \mid a^2 = b^3 = (ab)^5 = 1\rangle$
I_h	$A_5 \times C_2$	120	$\langle a, b, c \mid a^2 = b^3 = (ab)^5 = 1, ac = ca, bc = cb\rangle$
O	S_4	24	$\langle a, b \mid a^2 = b^3 = (ab)^4 = 1\rangle$
O_h	$S_4 \times C_2$	48	$\langle a, b, c \mid a^2 = b^3 = (ab)^4 = 1, ac = ca, bc = cb\rangle$
T	A_4	12	$\langle a, b \mid a^2 = b^3 = (ab)^3 = 1\rangle$
T_h	$A_4 \times C_2$	24	$\langle a, b, c \mid a^2 = b^3 = (ab)^3 = 1, ac = ca, bc = cb\rangle$
T_d	S_4	24	$\langle a, b \mid a^2 = b^3 = (ab)^4 = 1\rangle$
C_∞	$C_\infty = SO(2, R)$	∞	no finite presentation
$C_{\infty v}$	D_∞	∞	no finite presentation
$C_{\infty h}$	$C_\infty \times C_2$	∞	no finite presentation
D_∞	D_∞	∞	no finite presentation
$D_{\infty h}$	$D_\infty \times C_2$	∞	no finite presentation

Note that some of these groups are isomorphic, so they do not have any differences significant for mathematician, but are significantly different from a chemical point of view.

Let us concentrate first at the first eight groups in the above table. All of them are either dihedral, cyclic, products of two cyclic or products of dihedral and cyclic groups. In the above presentations, the element a denotes the rotation and the element b a symmetry or, in the case of C_i, inversion i.

- If there is just one generator, the group is cyclic C_n. In chemistry notation, the possibilities are C_n, C_{2n}, C_s and C_i.

- If there are two generators, a rotation a of order n and a reflection b, the group is either $C_n \times C_2$ or D_n. If the generators commute, then it is $C_n \times C_2$ and if they do not, the group is D_n.

  If b is the symmetry with respect to the horizontal plane, then a and b commute. In this case, the group is
  $$C_n \times C_2 = \langle a, b \mid a^n = 1, b^2 = 1, ba = ab\rangle.$$
  The chemistry notation for this group is C_{nh}.

If b is the reflection with respect to a vertical plane, then a and b do not commute and $ba = a^{-1}b$. In this case, the point group is dihedral

$$D_n = \langle a, b \mid a^n = 1, b^2 = 1, ba = a^{n-1}b \rangle.$$

In chemistry notation, the point group is C_{nv}, D_n or D_{nd}.

- If there are three generators: rotation a, symmetry with respect to a vertical plane b, and a symmetry with respect to the horizontal plane c, these generators satisfy exactly the relations of the following presentation, so the group is $D_n \times C_2$ (D_{nh} in chemical notation).

$$D_n \times C_2 = \langle a, b, c \mid a^n = b^2 = c^2 = 1, ba = a^{n-1}b, bc = cb, ac = ca \rangle$$

In practice, not all values of n are possible. In crystallography, the feasible values of n are only $n = 1$, 2, 3, 4, 6, due to the crystallographic restriction theorem. In its basic form, this theorem is the observation that the rotational symmetries of a crystal are limited to 2-fold, 3-fold, 4-fold, and 6-fold. This is strictly true for the mathematical formalism, but in the physical world quasicrystals occur with other symmetries, such as 5-fold. (find out more at wikipedia.org). So, there are just 32 crystallographic point groups.

Linear molecules. Let us turn our attention to the point groups of linear molecules. Although none of these groups has a finite presentation, we can still describe their elements.

To match the notation in chemistry, consider such molecule as standing **upright** so that the z-axis is the axis around which we can rotate the molecule model. We use the notation C_∞ to denote the group of all rotations around the z-axis. As the rotation for 360 degrees is the same as rotation for 0 degrees, this group is isomorphic to a group of all the angles represented on a unit *circle*. The addition of two angles corresponds to the composition of two corresponding rotations. In mathematics, this group is known as $SO(2, R)$. To follow notation in chemistry, we denote it by C_∞. If the group has more elements than these rotations, there are three possibilities.

- There is a reflection b with respect to the horizontal plane. If x is any rotation in C_∞, then $bx = xb$. Thus, the group is the direct product $C_\infty \times C_2$, or, using the chemistry notation, $C_{\infty h}$.

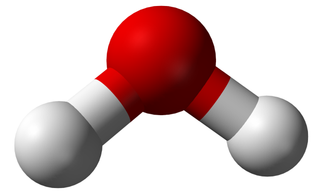
- There is a reflection b with respect to a vertical plane. If x is any rotation in C_∞, then $bx = x^{-1}b$. In this case, the groups is the infinite version of D_n which is denoted by D_∞ (or, using chemistry notation $C_{\infty v}$ or D_∞).

- There is a reflection b with respect to a vertical plane as well as a reflection c with respect to the horizontal plane. In this case, if x is any rotation in C_∞, then we have the following relations
$$c^2 = b^2 = 1, bx = x^{-1}b, cx = xc.$$
These relations define the group $D_\infty \times C_2$. This group is the infinite version of the group $D_n \times C_2$ and it is denoted by $D_{\infty h}$ in chemistry.

Examples.

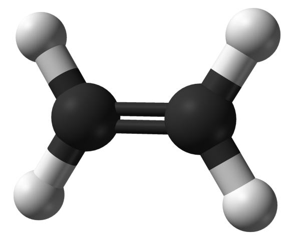
1. Water H_2O. This molecule has the following symmetries: identity 1, rotation for 180 degrees a, reflections with the respect to the vertical plane b, and their product ab. Note that ab is the reflection with respect to the horizontal plane. So, although the horizontal plane reflection is present also, it ends up being "expressible" via a and b only. Thus, this group has two generators and they commute. Hence, it is $C_2 \times C_2$.

You could also argue that, as a group with four elements, it has to be either $C_2 \times C_2$ or C_4. However, since the square of each nonidentity element is 1, it is not C_4 (recall that a^2 is not 1 in C_4). So, it is $C_2 \times C_2$. This group can be presented by



$$\langle a, b \mid a^2 = b^2 = 1, ba = ab\rangle.$$

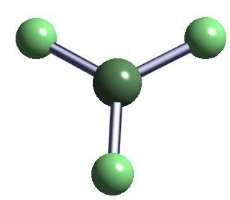
2. Ethylene C_2H_4. Let a be the rotation of the rectangle with the white atoms as its vertices for 180 degrees. Thus, $a^2 = 1$. There are reflections both with respect to the horizontal plane as well as with respect to vertical planes so there are two more generators b and c. Note that a commutes with both b and c (it commutes with b since $ba = a^{2-1}b = ab$). Thus, this group can be presented by



$$\langle a, b, c \mid a^2 = b^2 = c^2 = 1,\ ab = ba,\ ac = ca,\ bc = cb\rangle$$

Hence, this group is $C_2 \times C_2 \times C_2$. Note that this group has 8 elements: $1, a, b, ab, c, ac, bc, abc$. We can match these elements with the rotations with respect to all three coordinate axis, the inversion, the reflections with respect to one horizontal and two vertical planes and the identity.

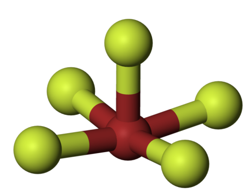
3. Boron trifluoride BF_3. If a denotes the rotation for 120, b the reflection with respect to a vertical plane and c the reflection with respect to the horizontal plane, then we have that $a^3 = 1, b^2 = c^2 = 1$, $ba = a^2b$, $ac = ca$, and $bc = cb$. Thus, this group can be presented by



$$\langle a, b, c \mid a^3 = 1, b^2 = 1, c^2 = 1, ba = a^2b, ca = ac, cb = bc\rangle$$

so it is $D_3 \times C_2$. Note that this group has 12 elements: 3 rotations $1, a, a^2$, three reflections with respect to the vertical planes b, ab, a^2b and six more elements $c, ac, a^2c, bc, abc, a^2bc$ which are compositions of these six with c.

4. Bromine Pentafluoride BrF_5. Four fluor atoms line in the same plane forming the vertices of a square. Bromine atom is in the center of that square and the remaining fluor atom is directly above the bromine.



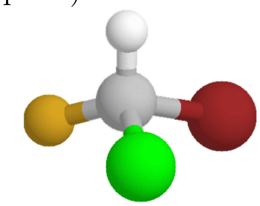
Because of that fifth fluor, there is no symmetry with respect to the horizontal plane.

Thus, if a is the rotation of the bottom square for 90 degrees and b is the reflection with respect to a vertical plane, then they generate the entire group. Since $a^4 = 1, b^2 = 1$ and $ba = a^3b \neq ab$, the group is noncommutative and can be presented by

$$\langle a, b \mid a^4 = 1, b^2 = 1, ba = a^3b\rangle$$

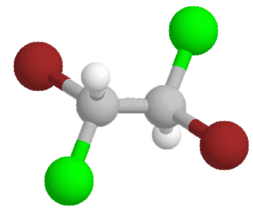
Thus, this is D_4, the group of symmetries of the bottom square (C_{4v} using the chemistry notation). It has eight elements, four rotations $1, a, a^2, a^3$ for 0, 90, 180 and 270 degrees respectively, and four reflections b, ab, a^2b, a^3b with respect to four vertical planes (xz and yz planes and two vertical planes passing the diagonals of the square).

5. CHFClBr. All five atoms are different, so just the trivial symmetry is present. Thus, the point group is the trivial (one element) group C_1.

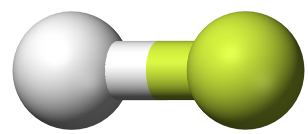


6. HClBrC-CHClBr. There is just one nontrivial operation: the inversion a with respect to the center. Since $a^2 = 1$, the group is

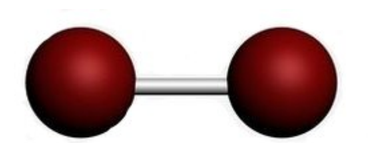
$$C_2 = \langle a \mid a^2 = 1 \rangle.$$



7. Hydrogen chloride HCl. If x is a rotation for any angle between 0 and 2π and b is the reflection with respect to a vertical plane (recall that we imagine this molecule standing "upright"), then x and b do not commute and the relations $b^2 = 1$ and $bx = x^{-1}b$ hold in this group. Thus, it is D_∞ ($C_{\infty v}$ using the chemistry notation).



8. Hydrogen H_2. Besides the rotations and the reflections with respect to vertical planes, there is also a reflection with respect to the horizontal plane (imagine this molecule standing "upright"). If x is any rotation, b a reflection with respect to a vertical plane and c the reflection with respect to the horizontal planes, then b and x do not commute and c commutes with both x and b. Thus, the relations $b^2 = c^2 = 1$, $bx = x^{-1}b$, $cx = xc$, and $cb = bc$ hold in this group and it is $D_\infty \times C_2$ ($D_{\infty h}$ using the chemistry notation).



There are many resources on the web detailing step-by-step process for finding the point group for any molecule and containing more examples of point groups and multimedia programs that helps you identify the point group of a given molecule. Feel free to explore those resources.

Practice Problems.

1. (a) Show that the set of real numbers different from $-\frac{1}{3}$ is a group under the following operation

$$a * b = a + b + 3ab.$$

(b) Determine whether it a group if $-\frac{1}{3}$ is included in the set.

2. Consider 2×2 matrices of the form $\begin{bmatrix} a & b \\ 0 & c \end{bmatrix}$ where a, b, c are real numbers with $a \neq 0$ and $c \neq 0$. These matrices are called **upper triangular invertible** matrices. Show that the set of such matrices with matrix multiplication is a group.

3. Write down the Cayley tables for the following groups.

   (a) $C_2 \times C_3$ (b) $C_2 \times C_2 \times C_2$ (c) D_5

4. The groups $C_8, C_4 \times C_2$ and $C_2 \times C_2 \times C_2, D_4$ have order 8. There is another group of order 8, called the **quaternion group**, usually denoted by Q, that can be presented by

$$\langle a, b \mid a^4 = 1, a^2 = b^2, ba = a^3 b \rangle.$$

   (a) Write down the Cayley table for this group and compare it with the Cayley tables for other two groups of order 8 generated by two elements: $C_4 \times C_2 = \langle a, b \mid a^4 = 1, b^2 = 1, ba = ab \rangle$, and $D_4 = \langle a, b \mid a^4 = 1, b^2 = 1, ba = a^3 b \rangle$.

   (b) Demonstrate that five groups of order 8, $C_8, C_4 \times C_2$ and $C_2 \times C_2 \times C_2, D_4$ and Q, are not isomorphic to each other.

5. Determine which of the following groups are isomorphic.

$$C_{36}, \quad C_{18} \times C_2, \quad C_{12} \times C_3, \quad C_9 \times C_4, \quad C_6 \times C_6,$$

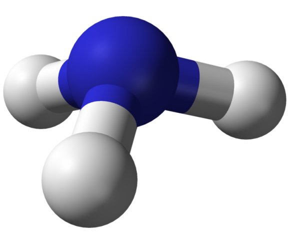
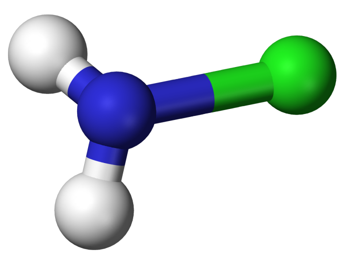
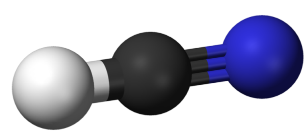
$$C_9 \times C_2 \times C_2, \quad C_6 \times C_3 \times C_2, \quad C_3 \times C_3 \times C_4, \quad C_3 \times C_3 \times C_2 \times C_2$$

6. Determine if the following pairs of groups are isomorphic. If they are, produce the isomorphism. If they are not, explain why.

   (a) C_3 and D_3.
   (b) C_6 and D_3.
   (c) S_3 and D_3.
   (d) S_n and D_n for $n > 3$.

7. Describe the point groups of the following molecules. Write down a presentation of the point group of each molecule and identify each group element as a symmetry operation.

   (a) Ammonia NH_3, (b) Chloramine NH_2Cl (c) Hydrogen cyanide HCN.

Solutions.

1. We need to check the four axioms A1 to A4.

A1. If a and b are real numbers different from $-\frac{1}{3}$, it is clear that the product $a*b = a+b+3ab$ is a real number but you need to check it is different from $-\frac{1}{3}$. Let us examine conditions on a and b that would make this product equal to $-\frac{1}{3}$.

$$a*b = a+b+3ab = -\frac{1}{3} \Rightarrow a+b+3ab+\frac{1}{3} = 0 \Rightarrow a+\frac{1}{3}+b(1+3a) = 0 \Rightarrow$$
$$a+\frac{1}{3}+3b(\frac{1}{3}+a) = 0 \Rightarrow (a+\frac{1}{3})(1+3b) = 0 \Rightarrow a+\frac{1}{3} = 0 \text{ or } 1+3b = 0 \Rightarrow a = -\frac{1}{3} \text{ or } b = -\frac{1}{3}.$$

This implication shows the contrapositive: if a and b are real numbers different from $-\frac{1}{3}$, then the product $a*b$ is also different from $-\frac{1}{3}$. Thus, the operation is closed.

A2. Check the associativity.

$$\begin{aligned}
(a*b)*c &= (a+b+3ab)*c \\
&= (a+b+3ab)+c+3(a+b+3ab)c \\
&= a+b+3ab+c+3ac+3bc+9abc \\
&= a+b+c+3ab+3ac+3bc+9abc \\
a*(b*c) &= a*(b+c+3bc) \\
&= a+(b+c+3bc)+3a(b+c+3bc) \\
&= a+b+c+3bc+3ab+3ac+9abc \\
&= a+b+c+3ab+3ac+3bc+9abc
\end{aligned}$$

Thus, the axiom A2 holds.

A3. To find the identity, you are looking for a number $x \neq \frac{-1}{3}$ with the property that $a*x = a$ and $x*a = a$ for every $a \neq \frac{-1}{3}$.

$$a*x = a \Rightarrow a+x+3ax = a \Rightarrow x+3ax = 0 \Rightarrow x(1+3a) = 0$$

Since $a \neq -\frac{1}{3}$, $1+3a \neq 0$ and we can cancel the equation $x(1+3a) = 0$ to get that $x = 0$. Thus, $a*0 = a$.

Check that $0*a = 0+a+3(0)a = a$ as well. Thus, the group identity element is 0.

A4. For any $a \neq \frac{-1}{3}$, you are looking for a number $x \neq \frac{-1}{3}$ with the property that $a*x = 0$ and $x*a = 0$.

$$a*x = 0 \Rightarrow a+x+3ax = 0 \Rightarrow x+3ax = -a \Rightarrow x(1+3a) = -a \Rightarrow x = \frac{-a}{1+3a}$$

Note that we can divide by $1+3a$ since $a \neq \frac{-1}{3}$. Check that $x*a = 0$ as well. Indeed $\frac{-a}{1+3a}*a = \frac{-a}{1+3a}+a+3a\frac{-a}{1+3a} = \frac{-a+(1+3a)a-3a^2}{1+3a} = \frac{-a+a+3a^2-3a^2}{1+3a} = \frac{0}{1+3a} = 0.$

(b) If we are considering the set of all real numbers instead of all numbers different from $\frac{-1}{3}$, then we do not get a group since the axiom A4 fails. Indeed, the equation $\frac{-1}{3}*x = 0$ has no solutions:

$$\frac{-1}{3}*x = 0 \Rightarrow \frac{-1}{3}+x+3(\frac{-1}{3})x = 0 \Rightarrow \frac{-1}{3}+x-x = 0 \Rightarrow \frac{-1}{3} = 0.$$

Thus, the element $\frac{-1}{3}$ does not have an inverse.

2. Check the four axioms.

A1. We need to show that the product of two upper triangular matrices with nonzero entries on the diagonal is again an upper triangular matrix with nonzero entries on the diagonal. Consider the matrices $\begin{bmatrix} a & b \\ 0 & c \end{bmatrix}$ and $\begin{bmatrix} p & q \\ 0 & r \end{bmatrix}$ with a, c, p, r non-zero.

$$\begin{bmatrix} a & b \\ 0 & c \end{bmatrix}\begin{bmatrix} p & q \\ 0 & r \end{bmatrix} = \begin{bmatrix} ap & aq+br \\ 0 & cr \end{bmatrix}$$

Thus, the product is again an upper triangular matrix. It is invertible since $ap \neq 0$ because both a and p are non-zero, and $cr \neq 0$ because both c and r are non-zero.

A2.

$$\left(\begin{bmatrix} a & b \\ 0 & c \end{bmatrix}\begin{bmatrix} p & q \\ 0 & r \end{bmatrix}\right)\begin{bmatrix} u & v \\ 0 & w \end{bmatrix} = \begin{bmatrix} ap & aq+br \\ 0 & cr \end{bmatrix}\begin{bmatrix} u & v \\ 0 & w \end{bmatrix} = \begin{bmatrix} apu & apv+(aq+br)w \\ 0 & crw \end{bmatrix}$$

$$\begin{bmatrix} a & b \\ 0 & c \end{bmatrix}\left(\begin{bmatrix} p & q \\ 0 & r \end{bmatrix}\begin{bmatrix} u & v \\ 0 & w \end{bmatrix}\right) = \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}\begin{bmatrix} pu & pv+qw \\ 0 & rw \end{bmatrix} = \begin{bmatrix} apu & a(pv+qw)+brw \\ 0 & crw \end{bmatrix}$$

The associativity holds since

$$apv+(aq+br)w = apv+aqw+brw \quad \text{and} \quad a(pv+qw)+brw = apv+aqw+brw.$$

A3. We need to find an invertible matrix $X = \begin{bmatrix} x & y \\ 0 & z \end{bmatrix}$ such that $AX = A$ for any invertible matrix $A = \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}$.

$$AX = A \Rightarrow \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}\begin{bmatrix} x & y \\ 0 & z \end{bmatrix} = \begin{bmatrix} a & b \\ 0 & c \end{bmatrix} \Rightarrow \begin{bmatrix} ax & ay+bz \\ 0 & cz \end{bmatrix} = \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}$$

This yields the equations $ax = a$, $ay + bz = b$ and $cz = c$. Since $a \neq 0$ and $c \neq 0$, the first and third equation give us $x = 1$ and $z = 1$. The second equation becomes $ay + b = b \Rightarrow ay = 0 \Rightarrow y = 0$ since $a \neq 0$. Thus we have that $X = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, the identity matrix. The equation $XA = A$ holds in this case as well.

If you suspected that the identity matrix is the identity element, you could just check that $A\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = A$ and $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}A = A$.

A4. Let I denote the identity matrix $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. For any given invertible matrix $A = \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}$, you are looking for an invertible matrix $X = \begin{bmatrix} x & y \\ 0 & z \end{bmatrix}$ such that $AX = I$ and $XA = I$.

$$AX = I \Rightarrow \begin{bmatrix} a & b \\ 0 & c \end{bmatrix}\begin{bmatrix} x & y \\ 0 & z \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \Rightarrow \begin{bmatrix} ax & ay+bz \\ 0 & cz \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

This yields the equations $ax = 1$, $ay + bz = 0$ and $cz = 1$. Since $a \neq 0$ and $c \neq 0$, the first and third equation give us $x = \frac{1}{a}$ and $z = \frac{1}{c}$. The second equation becomes $ay + b\frac{1}{c} = 0 \Rightarrow ay = \frac{-b}{c} \Rightarrow y = \frac{-b}{ac}$ since $a \neq 0$. Thus, $X = \begin{bmatrix} \frac{1}{a} & \frac{-b}{ac} \\ 0 & \frac{1}{c} \end{bmatrix}$. Check that XA is also equal to I.

3. (a) The table for $C_2 \times C_3$ can be found in the section on direct product of cyclic groups.
(b) $C_2 \times C_2 \times C_2 = \langle a, b, c \mid a^2 = b^2 = c^2 = 1, ab = ba, ac = ca, bc = cb\rangle$. The Cayley table is also displayed.
(c) $D_5 = \langle a, b \mid a^5 = 1, b^2 = 1, a^4b = ba\rangle$. Thus, this group consists of 10 elements: $1, a, a^2, a^3, a^4, b, ab, a^2b, a^3b, a^4b$.

	1	a	b	c	ab	ac	bc	abc
1	1	a	b	c	ab	ac	bc	abc
a	a	1	ab	ac	b	c	abc	bc
b	b	ab	1	bc	a	abc	c	ac
c	c	ac	bc	1	abc	a	b	ab
ab	ab	b	a	abc	1	bc	ac	c
ac	ac	c	abc	a	bc	1	ab	b
bc	bc	abc	c	b	ac	ab	1	a
abc	abc	bc	ac	ab	c	b	a	1

D_5	1	a	a^2	a^3	a^4	b	ab	a^2b	a^3b	a^4b
1	1	a	a^2	a^3	a^4	b	ab	a^2b	a^3b	a^4b
a	a	a^2	a^3	a^4	1	ab	a^2b	a^3b	a^4b	b
a^2	a^2	a^3	a^4	1	a	a^2b	a^3b	a^4b	b	ab
a^3	a^3	a^4	1	a	a^2	a^3b	a^4b	b	ab	a^2b
a^4	a^4	1	a	a^2	a^3	a^4b	b	ab	a^2b	a^3b
b	b	a^4b	a^3b	a^2b	ab	1	a^4	a^3	a^2	a
ab	ab	b	a^4b	a^3b	a^2b	a	1	a^4	a^3	a^2
a^2b	a^2b	ab	b	a^4b	a^3b	a^2	a	1	a^4	a^3
a^3b	a^3b	a^2b	ab	b	a^4b	a^3	a^2	a	1	a^4
a^4b	a^4b	a^3b	a^2b	ab	b	a^4	a^3	a^2	a	1

4. (a) The three Cayley tables for $C_4 \times C_2$, dihedral D_4 and the quaternion group Q are below. The first group differs from the latter two in the bottom half of the table. The differences between D_4 and Q are in the bottom right part of the table and they are highlighted in the table for Q.

$C_4 \times C_2$	1	a	a^2	a^3	b	ab	a^2b	a^3b
1	1	a	a^2	a^3	b	ab	a^2b	a^3b
a	a	a^2	a^3	1	ab	a^2b	a^3b	b
a^2	a^2	a^3	1	a	a^2b	a^3b	b	ab
a^3	a^3	1	a	a^2	a^3b	b	ab	a^2b
b	b	ab	a^2b	a^3b	1	a	a^2	a^3
ab	ab	a^2b	a^3b	b	a	a^2	a^3	1
a^2b	a^2b	a^3b	b	ab	a^2	a^3	1	a
a^3b	a^3b	b	ab	a^2b	a^3	1	a	a^2

D_4	1	a	a^2	a^3	b	ab	a^2b	a^3b
1	1	a	a^2	a^3	b	ab	a^2b	a^3b
a	a	a^2	a^3	1	ab	a^2b	a^3b	b
a^2	a^2	a^3	1	a	a^2b	a^3b	b	ab
a^3	a^3	1	a	a^2	a^3b	b	ab	a^2b
b	b	a^3b	a^2b	ab	1	a^3	a^2	a
ab	ab	b	a^3b	a^2b	a	1	a^3	a^2
a^2b	a^2b	ab	b	a^3b	a^2	a	1	a^3
a^3b	a^3b	a^2b	ab	b	a^3	a^2	a	1

Q	1	a	a^2	a^3	b	ab	a^2b	a^3b
1	1	a	a^2	a^3	b	ab	a^2b	a^3b
a	a	a^2	a^3	1	ab	a^2b	a^3b	b
a^2	a^2	a^3	1	a	a^2b	a^3b	b	ab
a^3	a^3	1	a	a^2	a^3b	b	ab	a^2b
b	b	a^3b	a^2b	ab	$\mathbf{a^2}$	$\mathbf{a}$	$\mathbf{1}$	$\mathbf{a^3}$
ab	ab	b	a^3b	a^2b	$\mathbf{a^3}$	$\mathbf{a^2}$	$\mathbf{a}$	$\mathbf{1}$
a^2b	a^2b	ab	b	a^3b	$\mathbf{1}$	$\mathbf{a^3}$	$\mathbf{a^2}$	$\mathbf{a}$
a^3b	a^3b	a^2b	ab	b	$\mathbf{a}$	$\mathbf{1}$	$\mathbf{a^3}$	$\mathbf{a^2}$

(b) Out of five groups of order 8, $C_8, C_4 \times C_2$ and $C_2 \times C_2 \times C_2, D_4$ and Q, the first three are abelian and the last two are not so none of the three abelian groups is isomorphic with two non-abelian groups. Furthermore, no abelian group is isomorphic to any other abelian group (because 4 and 2 have a common divisor 2 and so do 2,2,and 2). The groups D_4 and Q are not isomorphic because D_4 has 5 elements of order 2 and just 2 of order 4 and Q has 2 elements of order 2 and 5 elements of order 4.

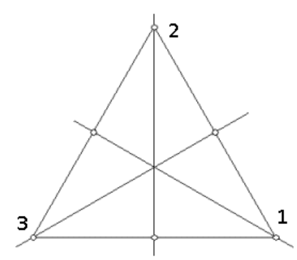
5. Note that $36 = 2^2 \cdot 3^2$ Since any power of 2 and any power of 3 do not have any common factor other than 1, $C_3 \times C_3$ can be combined with any of $C_2 \times C_2$ and C_4 creating isomorphic pairs of groups. Similarly, C_9 can be combined with any of $C_2 \times C_2$ and C_4. $C_3 \times C_3$ is not isomorphic to C_9 since 3 is a common factor of 3 and 3. Similarly, $C_2 \times C_2$ and C_4 are not isomorphic. Thus, there are four classes of abelian groups of order 36 such that the groups in same class are isomorphic and any two groups from two different classes are not isomorphic.

1.	$C_3 \times C_3 \times C_2 \times C_2$	$\cong C_6 \times C_3 \times C_2$	$\cong C_6 \times C_6$
2.	$C_3 \times C_3 \times C_4$	$\cong C_3 \times C_{12}$	
3.	$C_9 \times C_2 \times C_2$	$\cong C_{18} \times C_2$	
4.	$C_9 \times C_4$	$\cong C_{36}$	

6. (a) C_3 and D_3 are not isomorphic because one has 3 elements and the other has 6 elements.

   (b) C_6 and D_3 are not isomorphic because one is abelian and the other is not.

   (c) We show that S_3 and D_3 are isomorphic. Recall that $D_3 = \langle a, b \mid a^3 = 1, b^2 = 1, ba = a^2 b\rangle$ is the group of symmetries of the equilateral triangle. This group has six elements: the rotations $1, a, a^2$ (rotations for 0, 120 and 240 degrees respectively) and three



reflections b, ab, a^2b with respect to three axis as in the figure above. Recall also that S_3 has six elements represented by functions which map (1, 2, 3) to (1, 2, 3), (2, 3, 1), (3, 1, 2), (1, 3, 2), (3, 2, 1), and (2, 1, 3). Let us denote these 6 mappings by f_1 to f_6.

If we label the vertices of the triangle by 1,2,3 as on the figure below, we can see that the three rotations match the maps f_1, f_2 and f_3 exactly (also note that $f_2^3 = 1$, $f_2^2 = f_3$, and $f_2 f_3 = f_1$ which match the relations $a^3 = 1, aa = a^2$, and $aa^2 = 1$).

If we map b to f_4, then the product $f_2 f_4$ represents the composition of maps f_2 and f_4 that turns out to be the mapping $f_2 f_4 = (3, 2, 1) = f_5$. Thus, ab corresponds to f_5 Finally, the product $f_2^2 f_4 = f_2 f_5 = f_6$ so the element a^2b corresponds to f_6.

This demonstrates that the one-to-one mapping given by

1	a	a^2	b	ab	a^2b
f_1	f_2	f_3	f_4	f_5	f_6

of elements of D_3 onto the elements of S_3 preserves all the relations among the elements. Hence, it is an isomorphism.

Writing Cayley tables for these two groups produces the same tables that are a match further demonstrates the validity of this reasoning.

(d) S_n and D_n are not isomorphic for $n > 3$ because one has $2n$ and the other $n!$ elements. $n!$ is larger than $2n$ for $n > 3$.

7. (a) Ammonia. If a is the rotation for 120 degrees and b is the symmetry with respect to a vertical plane, then a and b do not commute and generate the entire group. The group satisfies the relations $a^3 = 1, b^2 = 1$, and $ba = a^2b$. Thus, it can be presented by $\langle a, b \mid a^3 = 1, b^2 = 1, ba = a^2b\rangle$ and so it is D_3 (C_{3v} for chemists). It has six elements, three rotations $1, a, a^2$ for 0, 120 and 240 degrees respectively, and three reflections with respect to three vertical planes (perpendicular to the plane of the triangle formed by the white atoms just as on the figure in the solution of the previous problem).

   (b) Chloramine NH_2Cl. The only non-identity group element is the reflection a fixing the green atom and switching the white atoms. Since $a^2 = 1$, the point group is $C_2 = \langle a \mid a^2 = 1\rangle$.

   (c) Hydrogen cyanide HCN. If x is a rotation for any angle between 0 and 2π and b is the reflection with respect to a vertical plane (recall that we imagine this molecule standing "upright"), then x and b do not commute and the relations $b^2 = 1$ and $bx = x^{-1}b$ hold in this group. Thus, it is D_∞ ($C_{\infty v}$ for chemists).