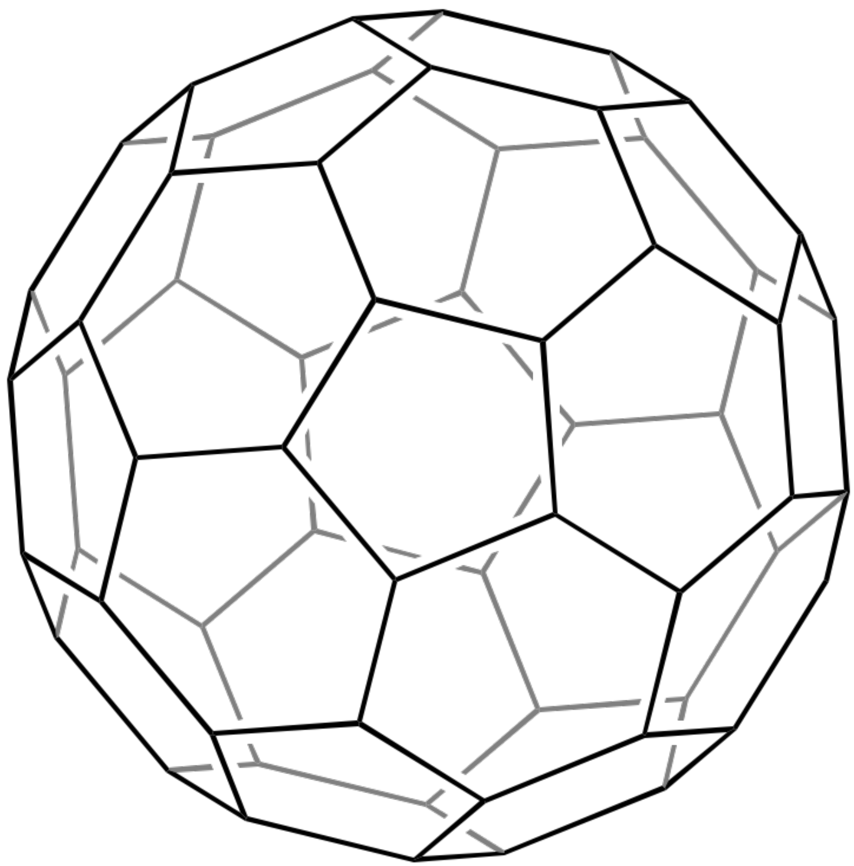
Fullerenes

In 1985 a group of chemists (Kroto, Heath, O'Brien, Curl, and Smalley) used laser irradiation to produce what was termed a "superstable" atom of 60 carbons, which they called the Buckminsterfullerene. Their proposed structure for this C_{60} molecule was the truncated icosahedron made of 60 vertexes which connect to form 12 pentagonal and 20 hexagonal faces.



This molecule is highly symmetrical, not just visually but in chemical terms as well, making it quite stable (which means it is less likely to react with other substances once formed). That said it doesn't quite have a chemical property called aromaticity, which would mean there was a complete delocalization of what are called π-electrons over the molecule and all of its bonds would be of equal length.

The primary bonds between atoms in a molecule are called σ bonds, but these bonds can be strengthened by double or triple bonds which are caused by π-electrons (forming π bonds). As a rule of thumb aromaticity can be determined by Hückel's rule, which says that planar cyclic molecules which have $4n + 2$ π-electrons, where $n = 0, 1, 2, \ldots$, are aromatic. This means that they are far less reactive than expected when compared to similar molecules. More recently a spherical version of Hückel's rule has been suggested, where aromaticity occurs when the number of π-electrons equals $2\,(n + 1)^2$. This formula was actually developed with C_{60} in mind to help understand the reactive properties of it, and other fullerenes.

Fullerenes, and related carbon structures like nanotubes, are important because they're quite strong and stable while still being able to conduct heat and energy well. Fullerenes can form cages around other molecules, like charged metal ions, which may be useful in the creation of more effective batteries and solar cells. C_{60} occurs naturally, often in soot with other carbon allotropes, and has even been discovered in a cloud of cosmic dust.

Beyond fullerenes

Even without these intriguing molecules group theory and the mathematics of symmetry are important topics that have shed light on many everyday phenomena. In chemistry, molecules are classified according to their symmetry. Furthermore, symmetries are used in orbital calculation and the determination of energy level of atoms or molecules. In materials science, the internal structures of crystals are determined by analyzing the two-dimensional x-ray projection of the atomic makeup of the crystal. Many games and puzzles, like the Rubik's cube, can be treated as permutation groups.

Groups

A group is made up of a set (which can be finite or infinite) and an operation. It is closed under that operation, meaning that when the operation is applied to any members of the group, the result is also a member of the group. Each group contains an identity element, usually denoted e, which is unique. When the identity element is applied (through the group's operation, such as addition or multiplication) to any other member of the group, that member is returned unaltered. For every element there is an inverse which takes that element to the identity, so if b is the inverse of a then $ab = e$. Furthermore, groups are associative, which means $(ab)\,c = a\,(bc)$.

The order of a group is the number of distinct elements it contains, written as $|G|$.

A few important groups

Z_n are the set of integers $\{0, 1, \ldots, n-1\}$ under addition mod n. For example $Z_5 = \{0, 1, 2, 3, 4\}$. Addition mod 5 means that $2 + 4 = 1$, since

$6 \; mod \; 5 = 1$. Zero is the identity element here.

D_n is the dihedral group of order $2n$. D_3 would be an equilateral triangle which can be reflected across its 3 axes of symmetry or rotated at 3 angles. The identity element here is rotation by 0°, denoted R_0.

$G =< a >$ is a cyclic group, which has an element that generates the whole group. For example $< 1 >$ can generate the entire group of $Z_5 = \{0, 1, 2, 3, 4\}$.

Subgroups

If a subset of a group, G, can be classed as a group in its own right under the operation of G then it's called a subgroup. This means that any product or inverse of the elements of the subgroup are also in that subgroup, as well as the identity element.

Permutation groups

A permutation group exchanges the elements of a group with each other. From a set of 3 elements $\{0, 1, 2\}$ we can easily count all of the possible permutations on the set using matrix notation. Since a permutation group is a group we know it contains an identity element

$$\varepsilon = \begin{bmatrix} 0 & 1 & 2 \\ 0 & 1 & 2 \end{bmatrix}$$

The first row contains the starting position of the three elements, while the second row shows where they are after ε is applied. This action can also be written in cycle notation which groups together the elements that exchange places under each action in parentheses.

For ε the cycle notation would be $\varepsilon = (0)\,(1)\,(2)$, however any cycle containing only one element can be omitted (since that element won't show up in any other segment of the cycle—each element can only appear once in order for the permutations to be bijections). Since eliminating all of the singular cycles might be ambiguous it's customary to just write one, so $\varepsilon = (0)$ is a correct and more succinct way to express the action ε. There are 6 possible permutations of $\{0, 1, 2\}$, listed below.

$\begin{bmatrix} 0 & 1 & 2 \\ 0 & 1 & 2 \end{bmatrix}$ $\varepsilon = (0)\,(1)\,(2)$	$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 0 \end{bmatrix}$ $\alpha = (012)$	$\begin{bmatrix} 0 & 1 & 2 \\ 2 & 0 & 1 \end{bmatrix}$ $\alpha^2 = (021)$
$\begin{bmatrix} 0 & 1 & 2 \\ 0 & 2 & 1 \end{bmatrix}$ $\beta = (12)\,(0)$	$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 0 & 2 \end{bmatrix}$ $\beta\alpha = (01)\,(2)$	$\begin{bmatrix} 0 & 1 & 2 \\ 2 & 1 & 0 \end{bmatrix}$ $\beta\alpha^2 = (02)\,(1)$

The collection of all possible permutations on a set is called the symmetric group of degree n, where n is the number of elements in the group being permuted, and represented by S_n. The group enumerated above is S_3.

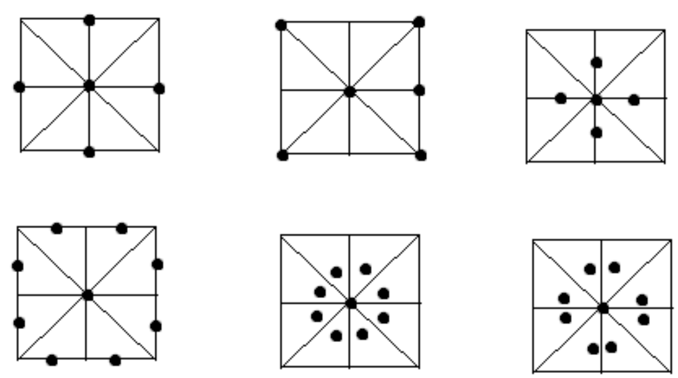
Every permutation can be broken down as the product of smaller cycles made of two elements each, called 2-cycles. For example ε can be broken into $(01)\,(01)$. This not unique, we could as easily have chosen $(12)\,(12)$, however what is unique is that every combination of 2-cycles we can compose for ε is even.

An important subgroup of any S_n is the set of its even permutations, called the alternating group of degree n and represented by A_n.

Rotations of a group

The stabilizer of a point is any permutation on a set that returns that point unchanged, denoted $|stab_G(a)|$, where a is the point. The orbit of a point, called $|orb_G(a)|$, is a permutation that moves a point a. This is easy to picture on a two dimensional plane. Let G be the rotations of a plane about a point P in the plane. Q is a point other than P on that same plane. The orbit of Q is the circle which is centered on P with a distance of $|PQ|$. The stabilizer of Q is a rotation of zero degrees, R_0.

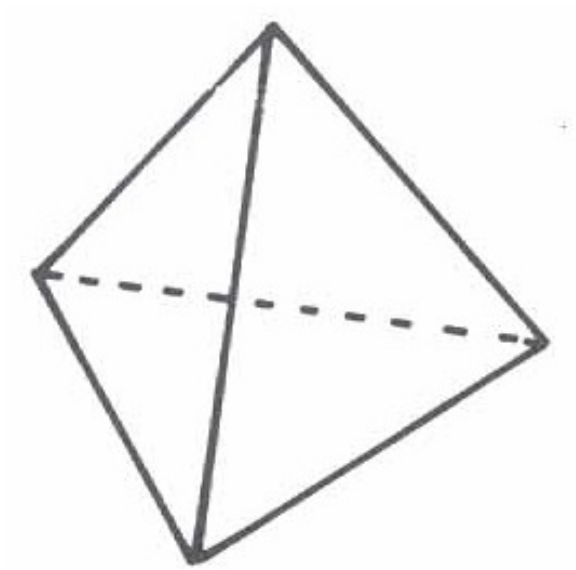
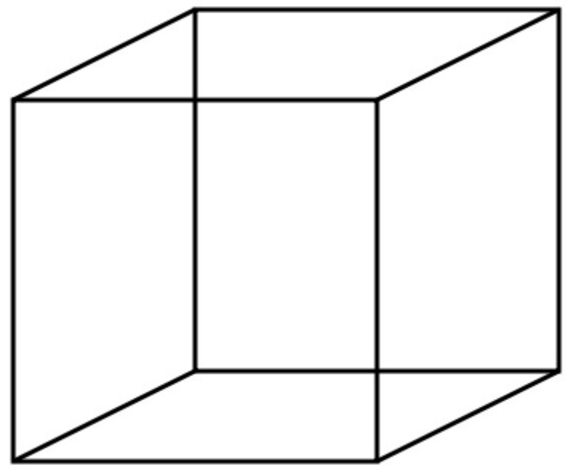
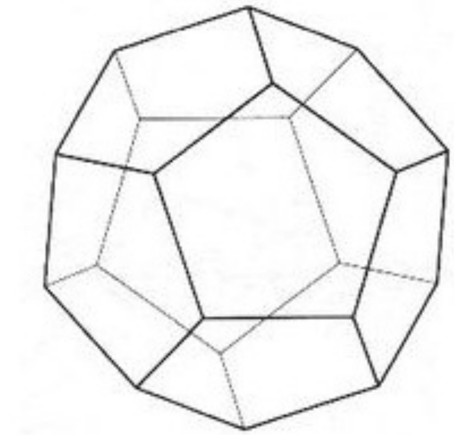
For example, D_4 acts a group of permutations of the square. For each square region, all the points are in the orbit of the square under D_4.



We'll also need to know Lagrange's theorem, which tells us that the order of a finite group G is divisible by the order of its subgroup H. Furthermore there are $|G|\,/\,|H|$ distinct left or right cosets of H in G. This leads us to the orbit-stabilizer theorem, which tells us that for any finite group of permutations on a set G, $|G|$ is given by $|orb_G\,(a)|\,|stab_G\,(a)|$, where a is any member of the set.

Often a group might have properties that seem familiar, and on close inspection we may realize it that we have seen these same properties in another group. If we determine that the elements of a group can be mapped to another group in a one-to-one fashion (that is, there is a dinstinct element for every member of the original group in the new group) in a way that preserves the operation of the group, then we say the two are isomorphic. Among other things, isomorphism preserves the order of a group.

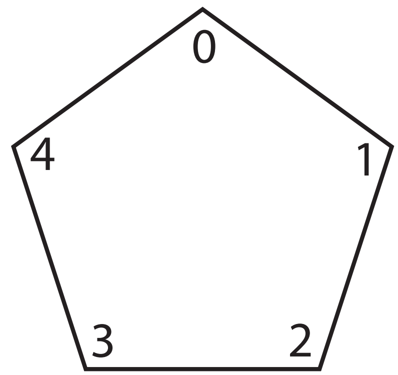
Up to isomorphism, the finite groups of rotations in $\mathbb{R}^3$ are Z_n, D_n, A_4, S_4 and A_5.

The group of rotations of a tetrahedron is isomorphic to A_4 with an order of 12. The group of rotations of a cube is isomorphic to S_4 with an order of 24. The group of rotations of a dodecahedron is isomorphic to A_5 with an order of 60.

The truncated icosahedron consists of 20 faces that are hexagons and 12 faces that are pentagons. If we let S be the set of 12 pentagons in the truncated icosahedron, labeled $\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$, we see that any pentagon can be carried to any other pentagon by some rotation. So for each element s there are 12 orbits, denoted $|orb\,(s)| = 12$. Next, there are five movements of rotation, $< R_{72^\circ} >$, which fix any particular pentagon so $|stab\,(s)| = 5$. If we let G be the whole group, then according to the orbit-stabilizer Theorem $|G| = |stab\,(s)| \cdot |orb\,(s)| = 60$.

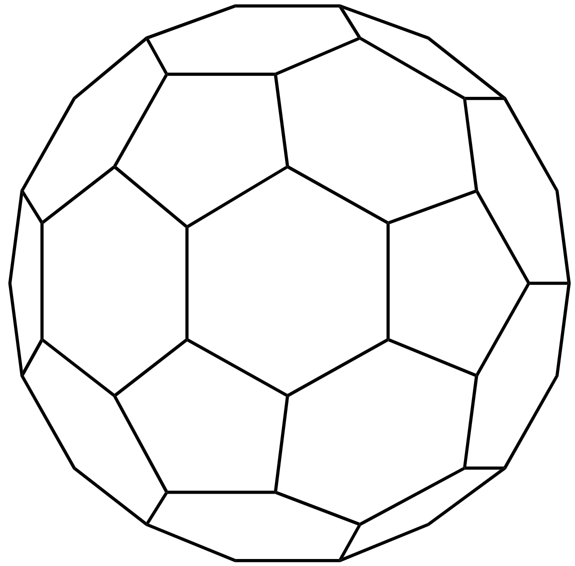
The group of rotations on the truncated icosahedron is isomorphic to A_5, the alternating group of degree 5. If we look at one of the pentagons



the rotations form a group C_5, generated by $< R_{72^\circ} >$.

In cyclic notation, as is used with permutation groups, we can say the set of rotations are $\{(0), (01234), (02413), (03142), (04312)\}$.

In the truncated icosahedron the rotations of the above graph forms a group of C_3.



According to the rules of the order of a permutation group, in A_5 we have the following cyclic groups: $<(134)>, <(024)>, <(013)>, <(124)>, <(014)>, <(123)>, <(012)>, <(234)>, <(034)>, <(023)>$. The total number of elements in all subgroups of C_3 is $\dfrac{5 \cdot 4 \cdot 3}{2} = 30$ and the number of subgroups of C_3 is $\dfrac{30}{3} = 10$.

Based on the properties of cosets (two left cosets of H are either identical or disjoint, and the left coset of H containing a does contain a), G can be formed by all distinct cosets of H (see Lagrange's theorem above).

If we let $H = \{(0), (01234), (02413), (03142), (04312)\}$

$$
\begin{aligned}
(0)H &= \{(0), (01234), (02413), (03142), (04312)\} \\
(134)H &= \{(134), (03124), (02143), (042), (01)(23)\} \\
(132)H &= \{(132), (034), (01243), (02)(14), (04231)\} \\
(123)H &= \{(123), (02134), (03)(24), (01432), (041)\} \\
(013)H &= \{(013), (03412), (02431), (142), (04)(23)\} \\
(024)H &= \{(024), (01423), (04132), (031), (12)(34)\} \\
(012)H &= \{(012), (02341), (13)(24), (03214), (043)\} \\
(234)H &= \{(234), (01324), (03)(14), (04312), (021)\} \\
(124)H &= \{(124), (02314), (04213), (032), (01)(34)\} \\
(143)H &= \{(143), (04)(12), (023), (01342), (03241)\} \\
(014)H &= \{(014), (04123), (02)(13), (03421), (243)\} \\
(01)(24)H &= \{(01)(24), (14)(23), (04)(13), (03)(21), (02)(34)\}
\end{aligned}
$$

Therefore, all the elements in the subgroups form the whole group of G and we verify that $|G|/|H| = 60/5 = 12$.

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