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Group theory and its applications to Chemistry

Dr CA Jyothirmayee&Dr K Sreelatha
Ch SD St Theresa's Autonomous college for women, ELURU

Abstract

Group Theory is the mathematical application of symmetry to an object to obtain knowledge of its physical properties. What group theory brings to the table, is how the symmetry of a molecule is related to its physical properties and provides a quick simple method to determine the relevant physical information of the molecule. The symmetry of a molecule provides you with the information of what energy levels the orbitals will be, what the orbitals symmetries are, what transitions can occur between energy levels, even bond order to name a few can be found, all without rigorous calculations. The fact that so many important physical aspects can be derived from symmetry is a very profound statement and this is what makes group theory so powerful.To a fully understand the math behind group theory one needs to take a look at the theory portion of the Group Theory topic.

Key words: Group theory, Topological and algebraic groups, Lie theory

Introduction:

In mathematics and abstract algebra, **group theory** studies the algebraic structures known as groups. The concept of a group is central to abstract algebra: other well-known algebraic structures, such as rings, fields, and vector spaces, can all be seen as groups endowed with additional operations andaxioms. Groups recur throughout mathematics, and the methods of group theory have influenced many parts of algebra. Linear algebraic groups and Lie groups are two branches of group theory that have experienced advances and have become subject areas in their own right.

Various physical systems, such as crystals and the hydrogen atom, may be modelled by symmetry groups. Thus group theory and the closely relatedrepresentation theory have many important applications in physics, chemistry, and materials science. Group theory is also central to public key cryptography.Mathematicians classify mathematics as a study of patterns and group theory is the study of symmetries, this says enough about the place of group theory at the heart of modern mathematics.

One of the most important mathematical achievements of the 20th centurywas the collaborative effort, taking up more than 10,000 journal pages and mostly published between 1960 and 1980,

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that culminated in a completeclassification of finite simple groups.The range of groups being considered has gradually expanded from finite permutation groups and special examples of matrix groups to abstract groups that may be specified through a representation by generators and relations.

Topological and algebraic groups

An important elaboration of the concept of a group occurs if G is endowed with additional structure, notably, of atopological space, differentiable manifold, or algebraic variety. If the group operations m (multiplication) and i(inversion),are compatible with this structure, i.e. are continuous, smooth or regular (in the sense of algebraic geometry) maps, then G becomes a topological group, a Lie group, or an algebraic group.[2]

The presence of extra structure relates these types of groups with other mathematical disciplines and means that more tools are available in their study. Topological groups form a natural domain for abstract harmonic analysis, whereas Lie groups (frequently realized as transformation groups) are the mainstays of differential geometry and unitaryrepresentation theory. Certain classification questions that cannot be solved in general can be approached and resolved for special subclasses of groups. Thus, compact connected Lie groups have been completely classified. [3] proposed a principle in which another NN yield input control law was created for an under incited quad rotor UAV which uses the regular limitations of the under incited framework to create virtual control contributions to ensure the UAV tracks a craved direction. Utilizing the versatile back venturing method, every one of the six DOF are effectively followed utilizing just four control inputs while within the sight of un demonstrated flow and limited unsettling influences. Elements and speed vectors were thought to be inaccessible, along these lines a NN eyewitness was intended to recoup the limitless states. At that point, a novel NN virtual control structure which permitted the craved translational speeds to be controlled utilizing the pitch and the move of the UAV. At long last, a NN was used in the figuring of the real control inputs for the UAV dynamic framework. Utilizing Lyapunov systems, it was demonstrated that the estimation blunders of each NN, the spectator, Virtual controller, and the position, introduction, and speed following mistakes were all SGUUB while unwinding the partition Principle.

Lie theory

A Lie group is a group that is also a differentiable manifold, with the property that the group operations are compatible with the smooth structure. Lie groups are named after Sophus Lie, who laid the foundations of the theory of continuoustransformation groups. The term groups de Lie first appeared in French in 1893 in the thesis of Lie's student Arthur Tresse.

Lie groups represent the best-developed theory of continuous symmetry of mathematical objects and structures, which makes them indispensable tools for many parts of contemporary mathematics, as well as for modern theoretical physics. They provide a natural framework for analysing the continuous symmetries of differential equations (differential Galois theory), in much the same way as permutation groups are used in Galois theory for analysing the discrete symmetries of algebraic equations. An extension of Galois theory to the case of continuous symmetry groups was one of Lie's principal motivations.

Connection of Groups and Symmetry

Given a structured object X of any sort, a symmetry is a mapping of the object onto itself which preserves the structure. This occurs in many cases, for example

1. If X is a set with no additional structure, a symmetry is a bijective map from the set to itself, giving rise topermutation groups.
2. If the object X is a set of points in the plane with its metric structure or any other metric space, a symmetry is abijection of the set to itself which preserves the distance between each pair of points (an isometry). The corresponding group is called isometry group of X.
3. If instead angles are preserved, one speaks of conformal maps. Conformal maps give rise to Kleinian groups, for example.
4. Symmetries are not restricted to geometrical objects, but include algebraic objects as well. For instance, the equationhas the two solutions . In this case, the group that exchanges the two roots is the Galois groupbelonging to the equation. Every polynomial equation in one variable has a Galois group, that is a certain permutation group on its roots.

The axioms of a group formalize the essential aspects of symmetry. Symmetries form a group: they are closed because if you take a symmetry of an object, and then apply another symmetry, the result will still be a symmetry. The identity keeping the object fixed is always a symmetry of an object. Existence of inverses is guaranteed by undoing the symmetry and the associativity comes from the fact that symmetries are functions on a space, and composition of functions are associative.

Frucht's theorem says that every group is the symmetry group of some graph. So every abstract group is actually the symmetries of some explicit object.The saying of "preserving the structure" of an object can be made precise by working in a category. Maps preserving the structure are

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then the morphisms, and the symmetry group is the automorphism group of the object in question.

Applications of group theory

Applications of group theory abound. Almost all structures in abstract algebra are special cases of groups. Rings, for example, can be viewed as abelian groups (corresponding to addition) together with a second operation (corresponding to multiplication). Therefore, group theoretic arguments underlie large parts of the theory of those entities.

Galois theory

Galois theory uses groups to describe the symmetries of the roots of a polynomial (or more precisely the automorphisms of the algebras generated by these roots). The fundamental theorem of Galois theory provides a link between algebraic field extensions and group theory. It gives an effective criterion for the solvability of polynomial equations in terms of the solvability of the corresponding Galois group. For example, S_5, the symmetric group in 5 elements, is not solvable which implies that the general quintic equation cannot be solved by radicals in the way equations of lower degree can. The theory, being one of the historical roots of group theory, is still fruitfully applied to yield new results in areas such as class field theory.

Algebraic topology

Algebraic topology is another domain which prominently associates groups to the objects the theory is interested in. There, groups are used to describe certain invariants of topological spaces. They are called "invariants" because they are defined in such a way that they do not change if the space is subjected to some deformation. For example, thefundamental group "counts" how many paths in the space are essentially different. The Poincaré conjecture, proved in 2002/2003 by Grigori Perelman, is a prominent application of this idea. The influence is not unidirectional, though. For example, algebraic topology makes use of Eilenberg–MacLane spaces which are spaces with prescribed homotopy groups. Similarly algebraic K-theory relies in a way on classifying spaces of groups. Finally, the name of the torsion subgroup of an infinite group shows the legacy of topology in group theory.

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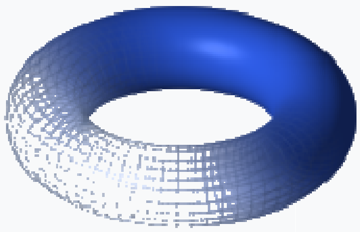
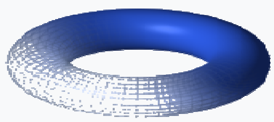


A torus. Its abelian group structure is induced from the map $\mathbf{C} \to \mathbf{C}/\mathbf{Z} + \tau\mathbf{Z}$, where τ is a parameter living in the upper half plane.



The cyclic group $\mathbf{Z}_{26}$underlies Caesar's cipher.

Algebraic geometry and cryptography

Algebraic geometry and cryptography likewise uses group theory in many ways. Abelian varieties have been introduced above. The presence of the group operation yields additional information which makes these varieties particularly accessible. They also often serve as a test for new conjectures.[9] The one-dimensional case, namely elliptic curves is studied in particular detail. They are both theoretically and practically intriguing.Very large groups of prime order constructed in elliptic curve cryptography serve for public-key cryptography. Cryptographical methods of this kind benefit from the flexibility of the geometric objects, hence their group structures, together with the complicated structure of these groups, which make the discrete logarithm very hard to calculate. One of the earliest encryption protocols, Caesar's cipher, may also be interpreted as a (very easy) group operation. In another direction, toric varieties are algebraic varieties acted on by a torus. Toroidalembeddings have recently led to advances in algebraic geometry, in particular resolution of singularities.

In chemistry, the symmetry of a molecule provides us with the information of what energy levels the orbitals will be, what the orbitals symmetries are, what transitions can occur between energy levels, even bond order and all of that is calculated using group theory.

Conclusion:

In chemistry and materials science, groups are used to classify crystal structures, regular polyhedra, and thesymmetries of molecules. The assigned point groups can then be used to determine physical properties (such aspolarity and chirality), spectroscopic properties (particularly useful for Raman spectroscopy, infrared spectroscopy, circular dichroism spectroscopy, magnetic circular dichroism spectroscopy, UV/Vis spectroscopy, and fluorescence spectroscopy), and to construct molecular orbitals.Molecular symmetry is responsible for many physical and spectroscopic properties of compounds and provides relevant information about how chemical reactions occur. In order to assign a point group for any given molecule, it is necessary to find the set of symmetry operations present on it. The symmetry operation is an action, such as a rotation around an axis or a reflection through a mirror plane. In other words, it is an operation that moves the molecule such that it is indistinguishable from the original configuration. In group theory, the rotation axes and mirror planes are called "symmetry elements". These elements can be a point, line or plane with respect to which the symmetry operation is carried out. The symmetry operations of a molecule determine the specific point group for this molecule.

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