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Symmetry as a Theme in Chemistry and Physics

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> ... *The one supreme difference between the scientific method and the artistic method is, roughly speaking, simply this - that a scientific statement means the same thing wherever and whatever it is uttered, and that an artistic statement means something entirely different, according to the relation in which it stands to its surroundings*
>
> — G.K. Chesterton "Robert Browning" Macmillan (1903)

Abstract

A lecture for students of chemistry and physics on the role of symmetry in the physical sciences. Different examples of symmetry and their applications to real world situations will be considered and illustrated by a few simple experimental demonstrations.

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Symmetry and the 1996 Chemistry Nobel Prize

Kungl. Vetenskapsakademien
The Royal Swedish Academy of Sciences

The Royal Swedish Academy of Sciences has decided to award **the 1996 Nobel Prize in Chemistry** jointly to

Professor Robert F. Curl, Jr., Rice University, Houston, USA,
Professor Sir Harold W. Kroto, University of Sussex, Brighton, UK.,
and
Professor Richard E. Smalley, Rice University, Houston, USA,

for their discovery of fullerenes

Symmetry and the Platonic Solids

1. The Platonic solids have long fascinated people from all walks of life and are one of the prime examples of symmetry and are of considerable importance in understanding the discovery of the remarkable structure of the fullerene C_{60}.
2. **Regular polygons** have all their sides and angles equal. Typically we have the equilateral triangle, square, pentagon, hexagon etc.
3. Only the equilateral triangle, square and hexagon can fill a plane with no gaps.
4. **Regular polyhedra** are made from regular polygons with all faces equal and their vertices are all alike.
5. There are only five regular polyhedrons, the tetrahedron, cube, octahedron, dodecahedron and icosahedron. Their principal characteristics are given in the table below:-

Characteristics of Regular Polyhedra

Name	Shape of Faces	Number of Faces	Number of Vertices	Number of Edges
Tetrahedron	Triangle	4	4	6
Cube	Square	6	8	12
Octahedron	Triangle	8	6	12
Dodecahedron	Pentagon	12	20	30
Icosahedron	Triangle	20	12	30

Inspection of the above table reveals a number of interesting features:

a. In every case the number of Vertices + the number of Faces = the number of Edges + 2. i.e.

$$\boxed{\mathbf{V + F = E + 2}}$$

which is Euler's theorem.

b. **Duality** The cube and the octahedron are **dual** to each other. Both have 12 edges. The cube has 6 faces and 8 vertices while the octahedron has 8 faces and 6 vertices. Likewise the dodecahedron and icosahedron are dual to one another. The tetrahedron is **self-dual**.

High Symmetry of Molecules and Viruses

Molecules are known that have structures representing all five of the regular polyhedra, most notably in the polyboranes. Many viruses exhibit the high symmetry of the icosahedron. In solids one cannot fill a space, periodically, with icosahedra or dodecahedra due to their inherent five-fold symmetry. This does not, however, preclude the possibility of distorted icosahedral or dodecahedral symmetry in solids as typified by trivalent rare earth ions in the lanthanum magnesium double nitrates.

Lifting Degeneracy in High Symmetry Fields

The icosahedral and dodecahedral symmetries are less than that of a sphere but greater than that of the cube or octahedron. In free space with spherical symmetry each set of $(2J+1)$ states $|JM>$ associated with a total angular momentum J are degenerate, that is they are associated with the same energy. Reduce the symmetry and in general the degeneracy will be, at least, partly reduced. Thus in an octahedral field the five-fold degenerate $d-$orbital splits into two sublevels of degeneracy 2 and 3, the so-called e and t orbitals. Not so for icosahedral or dodecahedral symmetries, the full five-fold degeneracy remains! Only when we get to $J \geq 3$ does the degeneracy start to be lifted. This gives the experimentalist an opportunity to see if the icosahedral or dodecahedral symmetries are exact or only approximate.

Truncating the Icosahedron

We have already noticed that the icosahedron and dodecahedron have 12 and 20 vertices respectively. It would be surprising, to say the least, if we could place more than one carbon atom at each vertex. But we need to create a structure involving 60 carbon atoms! A regular polyhedron is unable to be so accommodating. Recall, the icosahedron has twelve vertices and each vertex has five-fold symmetry. If I make a cut in the plane perpendicular to the vertex axis I will be replacing the vertex by a pentagonal face having five vertices. If I do this to each vertex in turn I will form 12 new pentagonal faces leading to a figure having 60 vertices! If I make my truncations symmetrically and evenly I find a figure characterised by 12 pentagons each surrounded by 6 hexagons leading to a highly symmetrical figure having 12 pentagonal faces and 20 hexagonal faces. This figure is known as the **truncated icosahedron**, but one example of changing a regular polyhedron by cutting the corners. These lead to the 13 Archimedian solids. The truncated icosahedron was the shape required to understand the structure of the C_{60} fullerene. Such a shape has been known of for many centuries and a nice illustration is given by Leonardo da Vinci (1509) in his illustrations to Luca Paciolo :*De Divina Proportione.* The possibility of there being a molecule $C_{60}H_{60}$ with a truncated icosahedron shape was already discussed in 1973 but the paper was unnoticed in the West. *Dokl. Akad. Nauk SSSR* **209** 610 (1973).

The truncated icosahedron is likely to be important in designing gravitational wave detectors - a truncated icosahedron is expected to be 56 times more sensitive than the more usual bar detectors. Furthermore, truncated icosahedra are technically easier to machine than bars or spheres - symmetry helps!

The Consequences of Symmetry

1. Restricts possibilities- Selection Rules.
2. Shortens calculations. e.g. It is much quicker to assume $NaCl$ crystals are cubic and calculate properties than to deduce its structure by an *abinitio* quantum calculation.
3. Every symmetry is associated with an impossible experiment.
4. Symmetries are always tentative - we can not be sure that a future experiment will reveal that the symmetry is only approximate.

Chiral Symmetry and Apples

1. Handedness plays a common role in nature, more often than not, in a violation of mirror symmetry. Thus the human heart is usually, though not always, found on the left-hand-side. In many shell-fish, such as welks, both left-handed and right-handed varieties occur but usually one occurs with much greater frequency than others as well-known in the oil prospecting industry.

2. The mirror image of our left-hand is our right-hand. Have a look in a mirror and your left-hand while holding your right-hand nearby. Observe the reflected image of your left-hand and compare it with your right-hand without reflection. Now try looking at your left-hand in a mirror holding you hand horizontal and perpendicular to the vertical mirror. Rotate your hand clockwise and observe the rotation in the mirror. Now place your hand vertically and again rotate your hand clockwise and observe it in the mirror.

3. Most people cut an apple in half by making a vertical cut, the more eccentric might cut the apple by making a horizontal cut noting that the centre of the apple exhibits five-fold symmetry. A still more eccentric approach is to combine both methods to produce two-halves that are either both left-handed or both right-handed. The two halves of a given apple are said to have the same chirality. However it is not possible to join half of one of the apples to half of the other if they have opposite chirality as I now demonstrate.

Non-Periodic Symmetries

1. It is well-known that one cannot tile a plane with regular pentagons - gaps occur. This then leads to failure to be able to fill a space with regular objects having a five-fold axis of symmetry and hence crystals cannot occur with exact five-fold symmetry.
2. However, it is possible to tile a plane with tiles in such a way that islands of five-fold symmetry occur even though there is no overall five-fold symmetry. This is best illustrated with the Penrose tiling I have prepared for you.
3. The Penrose tiling involves just two types of tiles, darts and kites, which are joined together subject to matching rules. In the illustration the tiles are put together so that colours match.

Packing of Spheres

1. An important problem in chemistry, physics, coding, and industry is the packing of spheres of the same size to produce the maximum possible density. In two-dimensions the problem is simple as can be seen by putting 24 coins into a 6x4 rectangle. But can one insert a 25th coin? The answer is yes if we do a hexagonal rather than square packing as demonstrated.

2. What about higher dimensions? The densest possible packing in eight dime4nsions was determined, independently, by an English lawyer and two Russians in the 1870's. Forming what is known as the E(8) lattice packing.

3. The packing in eight dimensions can be considered in terms of eight component vectors, starting with the eight unit vectors

$$
\begin{aligned}
e_1 &= (1,0,0,0,0,0,0,0) \\
e_2 &= (0,1,0,0,0,0,0,0) \\
e_3 &= (0,0,1,0,0,0,0,0) \\
e_4 &= (0,0,0,1,0,0,0,0) \\
e_5 &= (0,0,0,0,1,0,0,0) \\
e_6 &= (0,0,0,0,0,1,0,0) \\
e_7 &= (0,0,0,0,0,0,1,0) \\
e_8 &= (0,0,0,0,0,0,0,1)
\end{aligned}
$$

4. Starting with these eight vectors I can form 112 eight component vectors of the type
$$\pm\mathbf{e}_i \pm \mathbf{e}_j \quad i \neq j$$
and a further 128 eight component vectors of the type
$$\frac{1}{2}(\pm\mathbf{e}_1 \pm \mathbf{e}_2 \pm \mathbf{e}_3 \pm \mathbf{e}_4 \pm \mathbf{e}_5 \pm \mathbf{e}_6 \pm \mathbf{e}_7 \pm \mathbf{e}_8)$$
where the number of positive signs is *even*, otherwise all possible choices of signs are allowed. There are a total of 240 vectors each of length $\sqrt{2}$
5. Each vector defines a point in an eight dimensional space and each point can be associated with a unit sphere with each sphere touching all the others. Such a lattice finds practical applications in coding theory.
6. If we add eight null vectors $(0,0,0,0,0,0,0,0)$ to the above 240 non-null vectors we obtain precisely the root lattice of the exceptional Lie algebra $e(8)$ associated with the Lie group $E(8)$.

Higher Symmetries

1. The exceptional group $E(8)$ is but one example of the sort of Lie groups that physicists have become interested in making applications of ideas of symmetry. More common examples are the rotation group, $SO(3)$ and its covering group $SU(2)$, which are fundamental to the quantum theory of angular momentum. The group $SU(3)$ arises in the theory of strong interactions in particle physics and as the foundation group of quantum chromodynamics (QCD).
2. In general physicists strive to look for the highest possible symmetry group that can be used to describe a given system. The concern is not necessarily that the symmetries be "exact" but most commonly in studying how the symmetry is broken and ultimately makes contact with observable phenomena as measured by experiment. Nowhere is this seen more dramatically than in attempts to construct theories that seek to produce a unified theory of all interactions - strong, weak, electromagnetic, and gravity. The basic idea is that in the very early stages of the universe there was a single force field of exceptionally high symmetry and as the universe cooled the symmetry was broken and the various forces became distinct as we observe them today.

3. Much progress has come from people trying to extend and generalise the concept of symmetry. Thus in the 1970's people started to develop supersymmetry theories that tried to place bosons (integer spin particles) and fermions (half-integer spin particles) on and equal footing. This meant introducing operators that could turn a boson into a fermion and vice-versa. Remarkably such operators appeared to translate an object in space-time and hence in such theories gravity seemed natural and the concept of *supergravity* was born. Such theories seemed most natural in an eleven dimensional spacetime and it became common to speak of eleven dimensional supergravity. It was hoped that eleven dimensional supergravity could lead to a unified theory of forces however while certain particles appeared naturally in the theory, such as the massless spin 2 graviton and the photon, it did not encompass enough of particle physics to be an adequate superunified theory.
4. Prior to 1984 most physicists were totally unfamiliar with the exceptional group $E(8)$. In 1984 saw the beginning of the first "string revolution" with the publication of a key paper by Green and Schwarz on superstrings. Both classical and quantum physics has been plagued by unwelcome singularities and infinite divergences. These are usually associated with point particle interactions. In superstring theory the key idea was to combine the concept of supersymmetry with the concept of strings. The string concept replaced point objects by objects extended in one-dimension as in the case of a piece of string. This has the effect of "spread-

ing out" the interaction as shown in the figure. Green and Schwarz found that such theories were severely constrained and it appeared that the only consistent theories involved either the product group $SO(32)$ or $E(8) \times E(8)$. The disappointing feature was that there were two possibilities and not one unique possibility. Shortly thereafter other possible superstring theories were conceived and the possibility of a unique theory receded. The eleven dimensional supergravity was abandoned and ten-dimensional superstring theories became the vogue. The central problem seemed to be to compactify (or curl up) the extra dimensions to make contact with the "real" four-dimensional space-time world we inhabit and to make practical calculations using perturbation expansions. The latter problem has been especially severe and led to a stalemate in superstring theory.

The M-theory Revolution of 1995

1. The entire situation changed in mid-1995 heralding the second string revolution. I sketch only the briefest of details. This involved the discovery of new symmetries associated with superstring theories. Already startling results have appeared - in some cases calculations, previously beyond any supercomputer, have been reduced to pencil and paper calculations. All the various string theories turn out to be related and hence cannot be regarded as distinct theories but rather one theory becomes the limiting form of one of the other theories. The key idea is known as "*String Duality.*

2. Recall Maxwell's equations of electromagnetism, in the absence of sources, (i.e. currents and charges)

$$\nabla \cdot \mathbf{E} = 0 \quad \nabla \times \mathbf{E} + \dot{\mathbf{B}} = 0$$
$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \times \mathbf{B} - \dot{\mathbf{E}} = \mathbf{0}$$

   The equations are invariant under $\mathbf{E} \to \mathbf{B}, \quad \mathbf{B} \to -\mathbf{E}$ which exchanges electric and magnetic fields. This is an example of *duality symmetry.* If charged particles are added to the equations, the duality symmetry is only preserved only if *both* electric charges *and* magnetic monopoles.

3. The possible existence of magnetic momopoles was considered by Dirac leading to the quantization condition which relates the electric charge e to the magnetic charge g as, with $\hbar = 1$,

$$eg = 2\pi$$

In that case duality exchanges not only the electric and magnetic fields but also electric and magnetic charges. Since eg is fixed and $e \ll 1$ while $g \gg 1$ we can regard electrodynamics in terms of electric charges as a *weakly coupled* theory while if it was based upon magnetic charges it would be a *strongly coupled* theory and would require, unlike conventional QED, a very complicated and difficult non-perturbative treatment.

4. The M-theory revolution of 1995 is the recognition of the duality symmetry as a symmetry of string theory. The key idea is that the strongly coupled limit of any string theory is equivalent to the weakly coupled limit of some other string theory. Thus all string theories become connected and all are subsumed in an eleven-dimensional M-theory with the duality symmetry manifest. To atomic physicists the analogue can be seen in $LS-$coupling and $jj-$coupling. In $LS-$coupling the calculation of Coulomb matrix elements is "easy" while the calculation of spin-orbit interactions is "hard". Conversely in $jj-$coupling the calculation of Coulomb matrix elements is "hard" while the calculation of spin-orbit interactions is "easy".

5. The M-theory is developing very rapidly. One of the first applications has been in the application of quantum theory to black holes. Over the past 20 years it has been thought that one could not successfully combine quantum theory and general relativity in nthe description of black holes and hence some modification of quantum theory would be required. Calculations in the past few months, based upon the concept of duality and strings has shown that one can indeed give a consistent treatment of the quantum theoretical description of black holes without the need to modify the basic ideas of quantum theory.

Ultimate Symmetries

The developments of M-theory are startling and may indicate that we are on the path to the discovery of the ultimate symmetries of the laws of the universe. There is still a long way to go and history shows that it is always dangerous to assume we are reaching the end of the road

With the exciting experiments planned for the next century I am confident that it will be possible to make tremendous progress in understanding very basic properties of the universe, its past, present and future. Much imaginative and daring thought will be required with ultimate constraints coming from experiment, though significant areas will remain unverifiable as the energies that occurred in the very early universe will be forever beyond human possibilities. Poets, musicians, creators of great literature will all be required to express our story for our story is a never ending story. Finis...

... If you look at the history of 20th century physics, you will find that the symmetry concept as a most fundamental theme, occupying center stage in today's theoretical physics. We cannot tell what the 21st century will bring us but I feel safe to say that for the next twenty years many theoretical physicists will continue to try variations on the fundamental theme of symmetry at the very foundations of our theoretical understanding of the structure of the physical universe
— C. N. Yang *Chinese J. Phys.* **32**, 1437 (1994)

The only questions worth asking are the unanswerable ones
— John Ciardi *Saturday Review-World (1973)*

For every complex question there is a simple answer — and it's wrong.
— H. L. Mencken