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Symmetry in Formation of Molecules

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Abstact: *It is very important to understand the symmetry and point group of orbitals and molecules so that their behaviours under different circumstances are clearly understood. The point groups are based on the shapes of orbitals and structures of molecules. For example, s orbital is spherical and has a particular symmetry, while p orbital has dumbbell shape and has different symmetry. Similarly, d orbitals have different shapes and hence different symmetries. Methane has a tetrahedral shape and its symmetry is Td, while benzene is hexagonal planar and its symmetry is D6h. Water is V shaped and its point group is C_2V. In order to understand the splitting of orbitals in different environments and the spectral characteristics of complexes, their symmetries and point groups must be understood.*

Keywords - *Symmetry, Orbitals , Molecule, Shapes.*

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I. Introduction

You will as of now be acquainted with the idea of symmetry in a regular sense. In the event that we say something is 'symmetrical', we normally mean it has reflect symmetry, or 'left-right' symmetry, and would appear to be identical if seen in a mirror. Symmetry is likewise essential in science. A few atoms are unmistakably 'more symmetrical' than others, yet what outcome does this have, assuming any?

The point of this course is to give a methodical treatment of symmetry in chemical frameworks inside the mathematical system known as gathering hypothesis (the purpose behind the name will wind up obvious later on). When we have ordered the symmetry of an atom, amass hypothesis gives a ground-breaking set of apparatuses that furnish us with significant knowledge into huge numbers of its chemical and physical properties. A few uses of gathering hypothesis that will be shrouded in this course include:

i. Predicting whether a given particle will be chiral, or polar.
ii. Examining synthetic holding and envisioning atomic orbitals.
iii. Predicting whether a particle may retain light of a given polarization, and which spectroscopic advances might be energized on the off chance that it does.
iv. Investigating the vibrational movements of the atom.

You may well meet a portion of these subjects once more, potentially in more detail, in later courses (eminently Symmetry II, and for the all the more scientifically slanted among you, Supplementary Quantum Mechanics). In any case, they will be acquainted here with give you a genuinely wide prologue to the capacities and utilizations of gathering hypothesis once we have worked through the essential standards and 'apparatus' of the hypothesis.

II. Symmetry And Group Theory

What is symmetry?

In basic dialect we can state that a question has symmetry, in the event that it has some exceptional attributes, for example, satisfying plans, while we take a gander at it. For instance, when we see the phone posts or electric light posts, we say that there is symmetry since they are orchestrated in a straight line at meet separation. Thus, when we take a gander at the entryways of houses, they will seem symmetric in view of their outlines. Normally, our eyes will look at the outline on one portion of the entryway with that of the other half and on the off chance that they locate some trademark highlight, for example, identical representation or other, at that point we feel there is symmetry.

A suspension connects, a butterfly, the flower petal and so on are a few cases to demonstrate the satisfying plans and henceforth, they are symmetric.

Gathering Theory is a numerical strategy by which parts of atoms symmetry can be determined. The symmetry of a particle uncovers data about its properties (i.e., structure, spectra, extremity, chirality, and so on…).Clearly, the symmetry of the direct atom A-B-An is unique in relation to An A-B. In A-B-A the A-B securities are proportionate, however in An A-B they are most certainly not. Nonetheless, imperative parts of the symmetry of H_2O and CF_2C_{l2} are the same. This isn't evident without Group Theory.

Symmetry Operations/Elements

A particle or question is said to have a specific activity if that task when connected leaves the atom unchanged. Each activity is performed with respect to a point, line, or plane - called a symmetry element. There are 5 sorts of tasks.

1. Identity
2. n-Fold Rotations
3. Reflection
4. Inversion
5. Improper n-Fold Rotation

1. Identity: is shown as E does nothing, has no impact all particles/objects have the personality task, i.e., forces E.

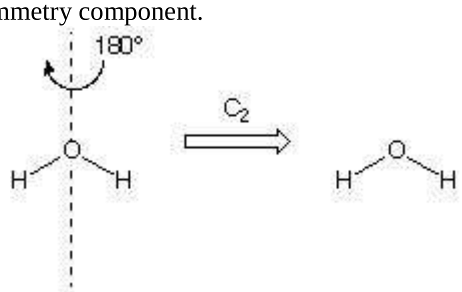
E has an indistinguishable significance from the number 1 does in duplication (E is required with a specific end goal to characterize inverses).

2. n-Fold Rotations: Cn, where n is a whole number pivot by 360°/n about a specific hub characterized as the n-overlay turn hub.

C_2 = 180° pivot, C_3 = 120° turn, C_4 = 90° revolution, C_5 = 72° pivot, C_6 = 60° pivot, and so forth.

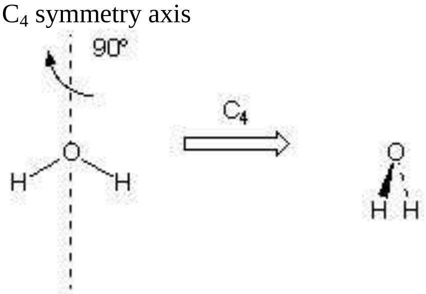
Revolution of H_2O about the hub appeared by 180° (C_2) gives a similar atom back.

Subsequently H_2O have the C_2 symmetry component.

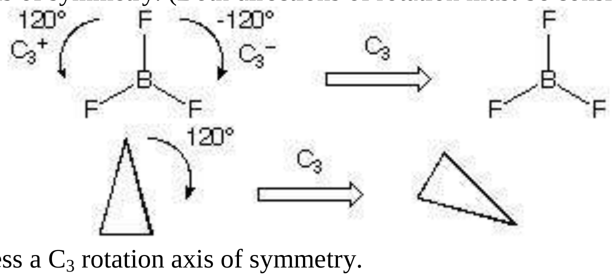


However, rotation by 90° about the same axis does not give back the identical molecule

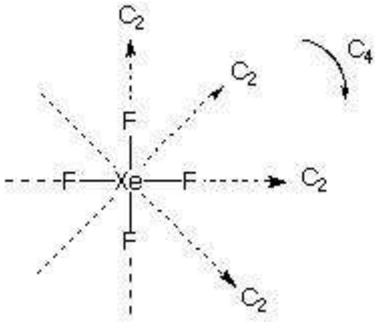
Therefore H_2O does NOT possess a C_4 symmetry axis



BF_3 posses a C_3 rotation axis of symmetry. (Both directions of rotation must be considered)



This triangle does not possess a C_3 rotation axis of symmetry.

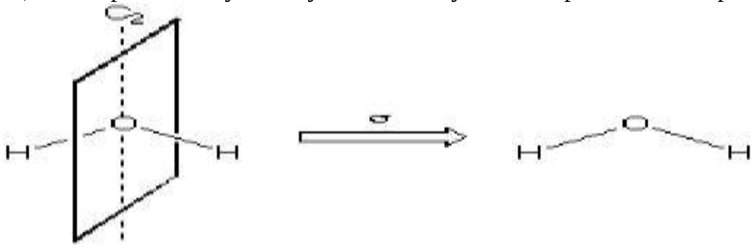


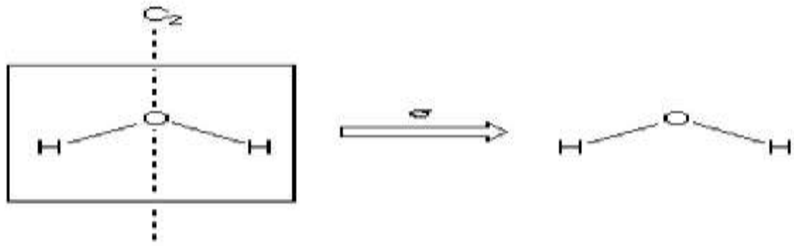
XeF_4 is square planar. It has four DIFFERENT C_2 axes

It also has a C_4 axis coming out of the page called the principle axis because it has the largest n. By convention, the principle axis is in the z-direction.

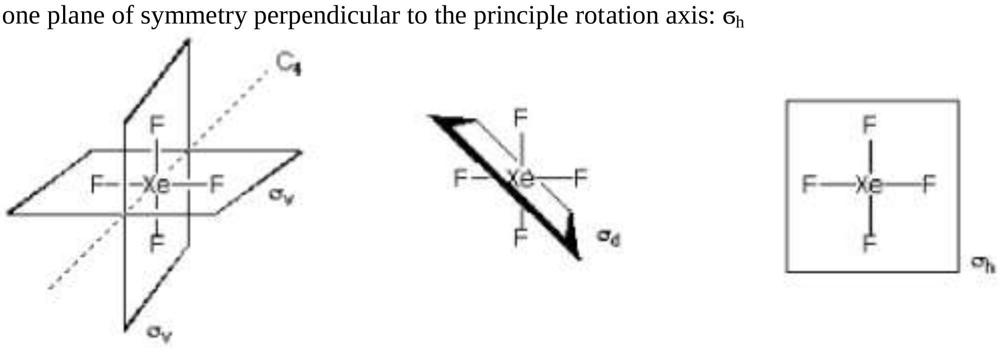
3. Reflection: σ(the symmetry element is called a mirror plane or plane of symmetry)

- If reflection about a mirror plane gives the same molecule/object back than there is a plane of symmetry (σ).
- If plane contains the principle rotation axis (i.e., parallel), it is a vertical plane (σ_v).
- If plane is perpendicular to the principle rotation axis, it is a horizontal plane (σ_h)
- If plane is parallel to the principle rotation axis, but bisects angle between 2 C_2 axes, it is a diagonal plane (σ_d)
- H2O posses 2 σ_v mirror planes of symmetry because they are both parallel to the principle rotation axis (C_2)



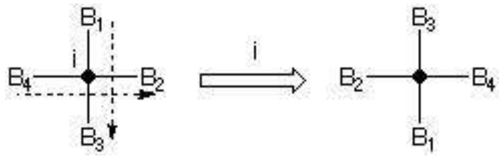


XeF_4 has two planes of symmetry parallel to the principle rotation axis: σ_v XeF_4 has two planes of symmetry parallel to the principle rotation axis and bisecting the angle between 2 C_2 axes : σ_d
XeF4 has one plane of symmetry perpendicular to the principle rotation axis: σ_h



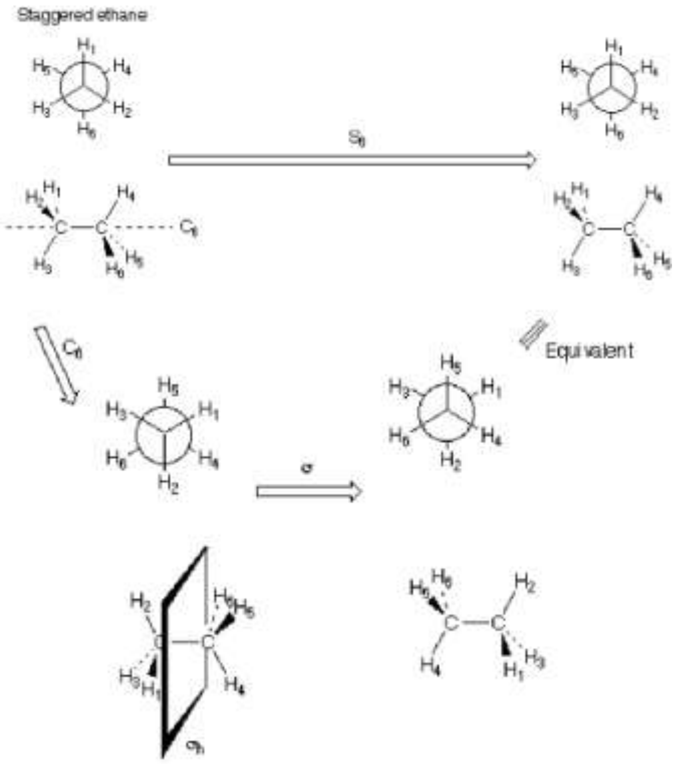
4. Inversion: i (the element that corresponds to this operation is a center of symmetry or inversion center)

The operation is to move every atom in the molecule in a straight line through the inversion center to the opposite side of the molecule.



Therefore XeF_4 posses an inversion center at the Xe atom.

5. Improper Rotations: Sn
n-fold rotation followed by reflection through mirror plane perpendicular to rotation axis
Note: n is always 3 or larger because S1 =σ and S2 = i.



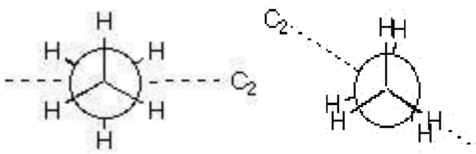
These are different, therefore this molecule does not possess a C_3 symmetry axis.

This molecule posses the following symmetry elements:

C_3, 3 σ_d, i, 3 $\perp$ C_2, S_6 . There is no C_3 or σ_h.

Eclipsed ethane posses the following symmetry elements:

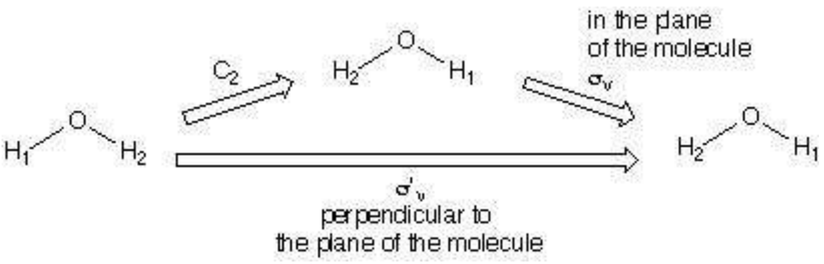
C_3, 3 σ_v, 3 $\perp C_2$, S_3, σ_h. There is no S_6 or i.



Compiling all the symmetry elements for staggered ethane yields a Symmetry Group called D_3d.
Compiling all the symmetry elements for eclipsed ethane yields a Symmetry Group called D_3h.
Symmetry group designations will be discussed in detail shortly
To be a group several conditions must be met:

1. Any result of two or more operations must produce the same result as application of one operation within the group.

i.e., the group multiplication table must be closed Consider H_2O which has E, C_2 and 2 σ_v's.



i.e., $\hat{C}_2\hat{\sigma}_v \equiv \hat{\sigma}'_v$ of course etc…

The group multiplication table obtained is therefore:

	E	C_2	σ_v	σ'_v
E	E	C_2	σ_v	σ'_v
C_2	C_2	E	σ'_v	σ_v
σ_v	σ_v	σ'_v	E	C_2
σ'_v	σ'_v	σ_v	C_2	E

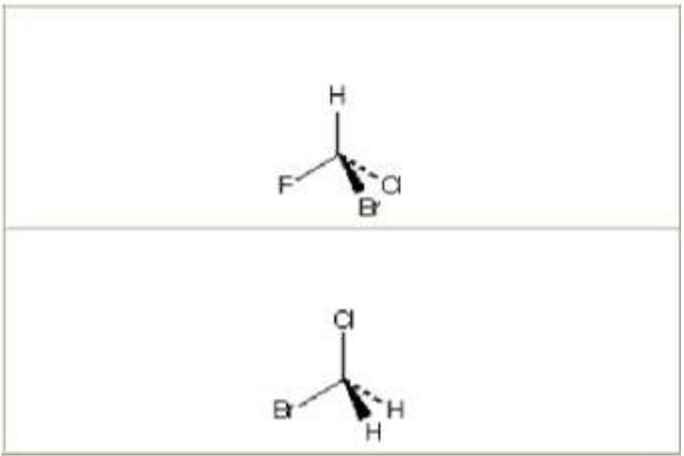
Note: the table is closed, i.e., the result of two operations is an operation in the group.
2. Must have an identity ($\hat{E}$)
3. All elements must have an inverse
i.e., for a given operation ($\hat{A}$) there must exist an operation ($\hat{B}$) such that $\hat{A}\,\hat{B} = \hat{E}$

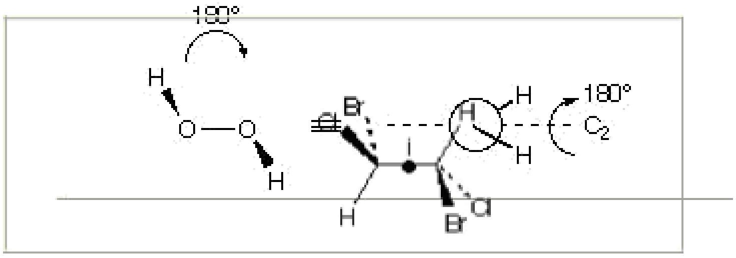
Classification of the Symmetry of Molecules

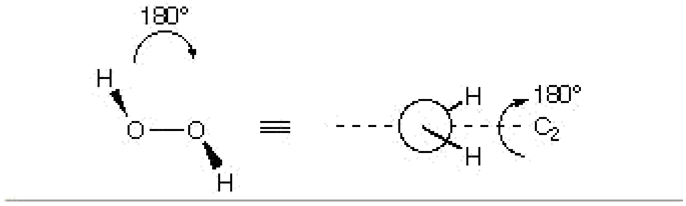
Certain symmetry operations can be present simultaneously, while others cannot. There are certain combinations of symmetry operations which can occur together. Symmetry Groups combine symmetry operations that can occur together. Symmetry groups contain elements and there mathematical operations.
For example, one of the symmetry elements of H_2O is a C_2-axis. The corresponding operation is rotation of the molecule by 180° about an axis.

Point Groups

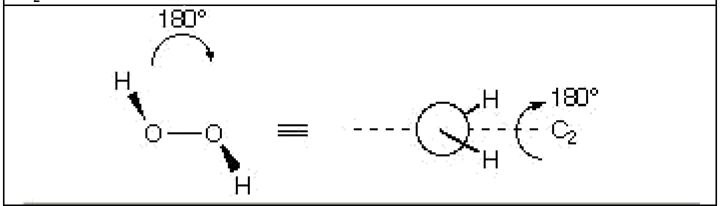
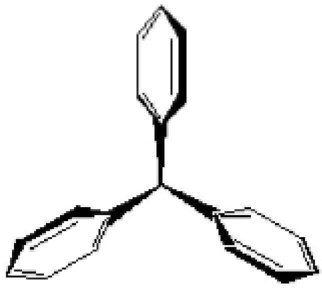
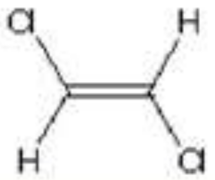
Low Symmetry Groups



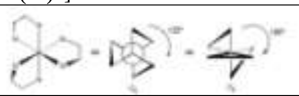
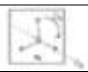


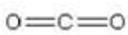


Cn, Cnv, Cnh Groups

Cn, Cnv, Cnh Groups
Cn: E and Cn only
C_2:


Cnv: E and Cnand nσv's
C2v: E, C2, 2σ_vH2O
C3v: E, C3, 3σ_vNH3
C.V: E, C., . σ_v HF, HCN
Cnh: E and Cnandσ_h(and others as well)


Dn, Dnv, Dnh Groups

Dn: E, Cn, n C_2axes⊥to Cn
D3: E, C_3, 3⊥C_2
[Co(en)3]$^{3+}$

D_nh: E, Cn, n C_2axes⊥to Cnσ_h
D_3h: E, C_3, 3⊥C_2,σ_h


D. h: E, C.,. ⊥C2,.h  H2

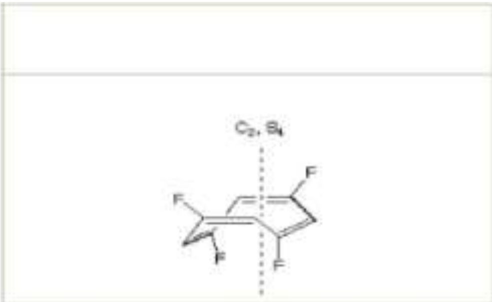
Dnd: E, Cn, n C2axes⊥to Cn,
D3d: E, C3, 3⊥C2, 3σ_d staggered ethane

S_n Group

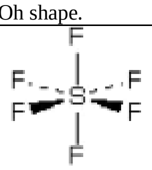
S_{2n}: E, Cn, S2n(no mirror planes)

S4, S6, S8, etc. (Note: never S3, S5, etc.)

S4: E, C2, S4



High Symmetry Cubic Groups, Td, Oh, Ih

Td: E, 8 C3, 3 C2, 6 S4, 6σ_d Tetrahedral structures No need to identify all the symmetry elements - simply recognize Td shape methane, CH_4
Oh: E, 8 C_3, 6 C_2, 6 C_4, i, 6 S_4, 8 S_6, 3σ_h, σ_d Octahedral structures No need to identify all the symmetry elements - simply recognize Oh shape.

Ih: E, 12 C5, 20 C3, 15 C2, i, 12 S10, 20 S6,
Icosahedron
Other rare high symmetry groups are **T**, **Th**,**O**, and **I**

Reference

[1]. P.K.Bhattacharya, Group Theory and its chemical appl‘ , Himalaya Pub. House.2005
[2]. B.K. Sharma, Spectroscopy, Goel Publishing House, Meerut, 2006.
[3]. Chatwal & Anand , Spectroscopy, Himalaya Pub. House.
[4]. Ira N Levine, Physical Chemistry,The McGraw-Hills Companies,2010.
[5]. P.W. Attkins, Physical Chemistry, The English Language Book Society, Oxford University Press (Elbs), London, 1982.
[6]. P.L. Soni, A Text Book Of Physical Chemistry, Sultan Chand And Sons, New Delhi, 1977.
[7]. Puri And Sharma, Principles Of Physical Chemistry, Shobhanlal Nagin Chand And Co., Jalandhar, 1988.
[8]. Gupta And Sharma, Physical Chemistry, K.Nath And Co., Meerut, 1987
[9]. Snehi (Hemant), Comprehensive Physical Chemistry, Pragati Prakashan, 1978
[10]. Gurdeep Raj, Advanced Physical Chemistry, Goel Publishing House, Meerut, 2009.
[11]. https://nptel.ac.in/courses/104106063/Module%201/Lectures%201-3/Lectures%201-3.pdf
[12]. http://www.bhojvirtualuniversity.com/slm/mscche1p4.pdf
[13]. https://www.thenakedscientists.com/articles/features/importance-symmetry
[14]. http://chemistry.rutgers.edu/undergrad/chem207/SymmetryGroupTheory.html

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